



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:09 PM UTC

PDB ID : 4K24 / pdb_00004k24
Title : Structure of anti-uPAR Fab ATN-658 in complex with uPAR
Authors : Huang, M.D.; Xu, X.; Yuan, C.
Deposited on : 2013-04-08
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

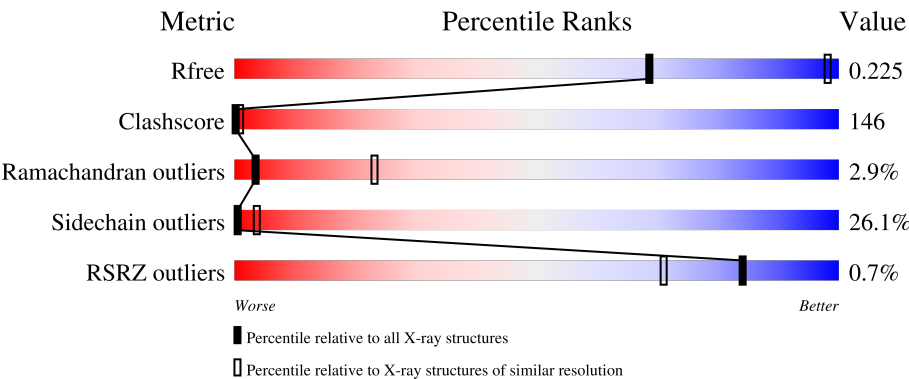
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	% 7%47%33%5%7%
2	B	40	10%55%30%5%
3	H	228	% 11%53%25%•7%
4	L	219	14%65%20%•
5	U	283	% 16%52%27%••

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Mol	Chain	Length	Quality of chain
6	C	2	 50% 50%
6	D	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	1	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			987	608	187	178	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP P00749
A	0	SER	-	expression tag	UNP P00749

- Molecule 2 is a protein called Vitronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	S	0	0	0
			312	185	51	68	8			

- Molecule 3 is a protein called anti-uPAR antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1606	1019	263	317	7			

- Molecule 4 is a protein called anti-uPAR antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	218	Total	C	N	O	S	0	0	0
			1690	1059	284	341	6			

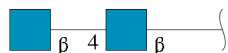
- Molecule 5 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	273	Total	C	N	O	S	0	0	0
			2095	1253	388	420	34			

There are 2 discrepancies between the modelled and reference sequences:

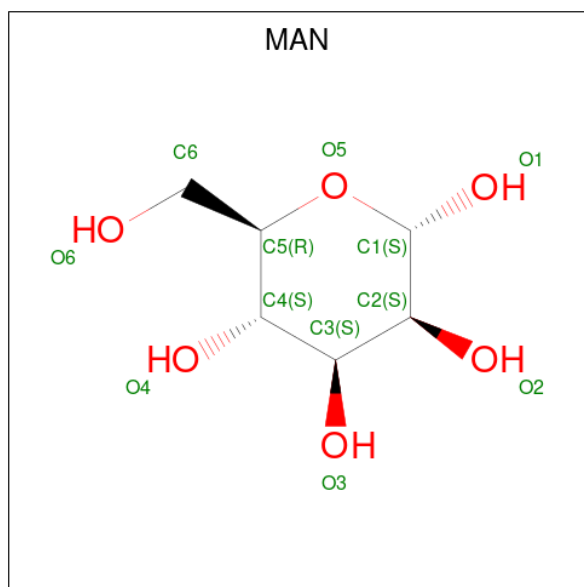
Chain	Residue	Modelled	Actual	Comment	Reference
U	-1	ARG	-	expression tag	UNP Q03405
U	0	SER	-	expression tag	UNP Q03405

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



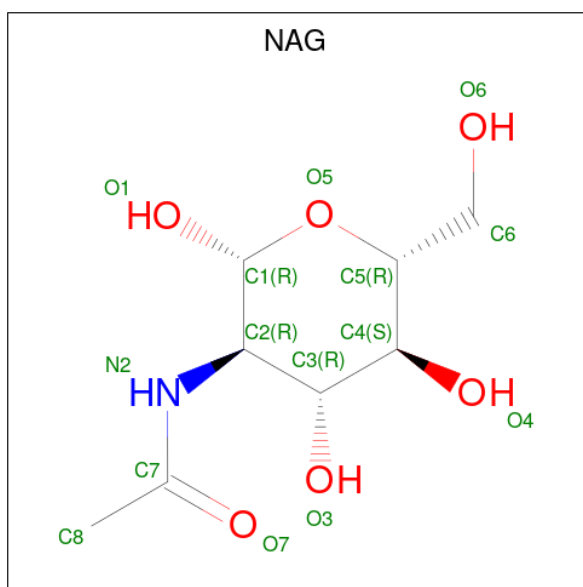
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	U	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

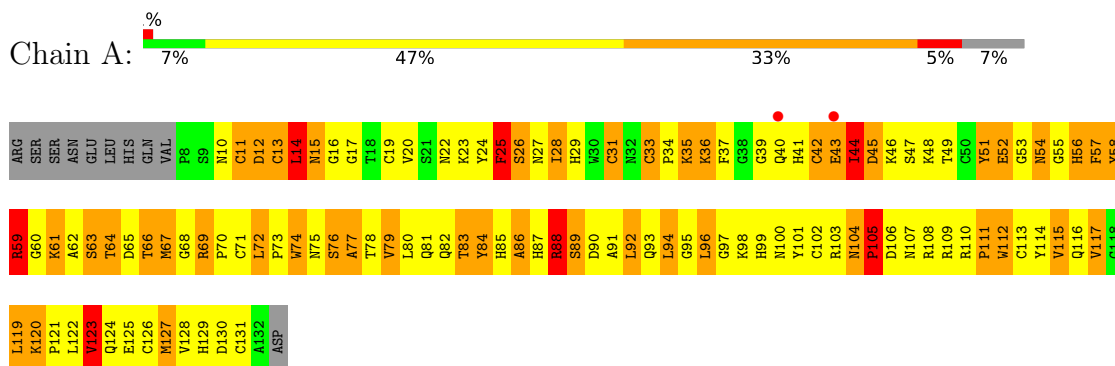


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	U	1	14	8	1	5	0	0

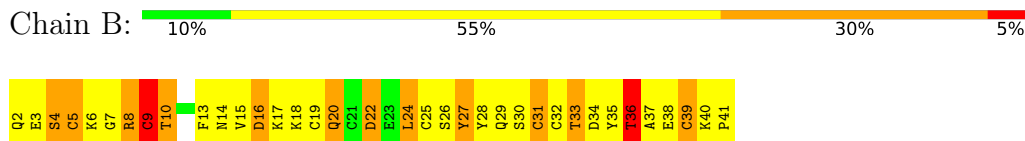
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

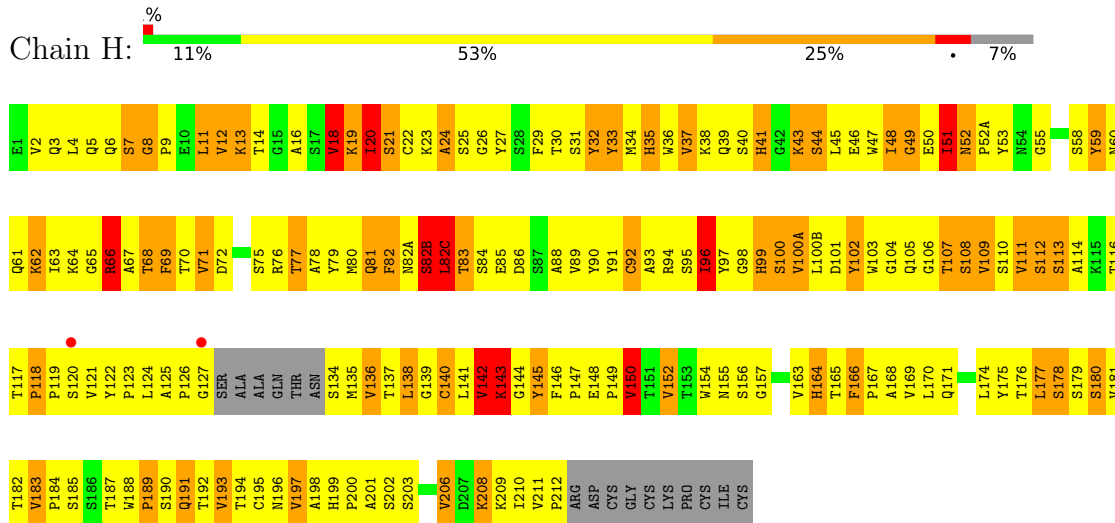
- Molecule 1: Urokinase-type plasminogen activator



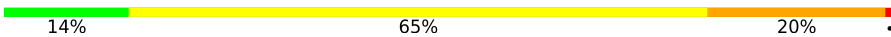
- Molecule 2: Vitronectin

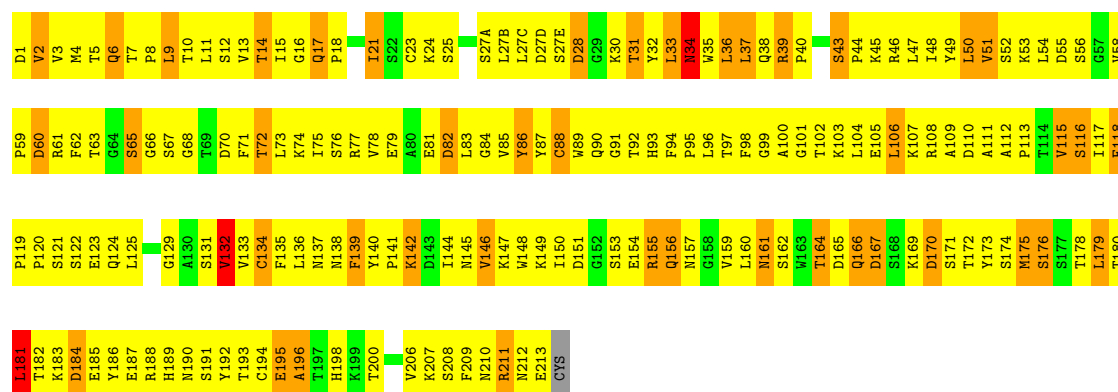


- Molecule 3: anti-uPAR antibody, heavy chain



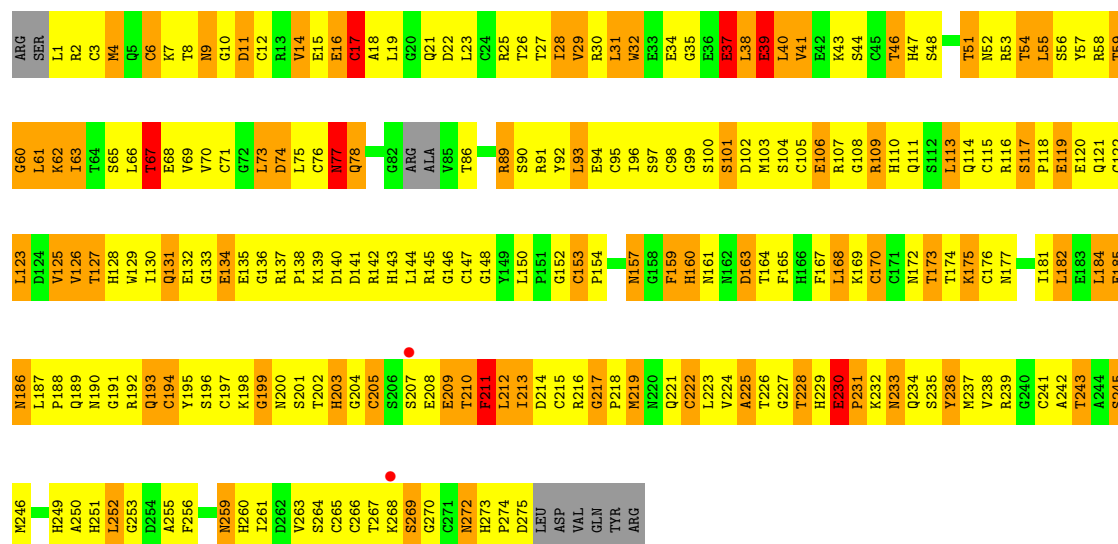
- Molecule 4: anti-uPAR antibody, light chain

Chain L: 



• Molecule 5: Urokinase plasminogen activator surface receptor

Chain U: 



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	164.66Å 164.66Å 391.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.90 – 4.50 26.90 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (26.90-4.50) 90.4 (26.90-4.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 4.41Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.217 , 0.275 0.225 , 0.225	Depositor DCC
R_{free} test set	622 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	171.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 493.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.028 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.046 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6771	wwPDB-VP
Average B, all atoms (Å ²)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	1/1015 (0.1%)	1.53	23/1372 (1.7%)
2	B	0.75	0/316	1.16	1/421 (0.2%)
3	H	0.92	2/1650 (0.1%)	1.46	37/2253 (1.6%)
4	L	0.71	0/1727	1.25	17/2346 (0.7%)
5	U	0.77	0/2129	1.35	32/2867 (1.1%)
All	All	0.82	3/6837 (0.0%)	1.37	110/9259 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
3	H	0	1
5	U	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	51	ILE	CA-CB	-8.81	1.46	1.55
1	A	123	VAL	CA-CB	-6.64	1.46	1.54
3	H	59	TYR	CA-C	-5.40	1.46	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	166	PHE	CA-C-N	14.19	135.11	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	166	PHE	C-N-CA	14.19	135.11	119.93
1	A	59	ARG	N-CA-C	-10.34	93.84	109.86
3	H	83	THR	N-CA-C	10.26	123.58	108.60
5	U	39	GLU	N-CA-C	9.85	123.59	108.42
5	U	217	GLY	CA-C-N	9.65	131.90	119.84
5	U	217	GLY	C-N-CA	9.65	131.90	119.84
5	U	117	SER	CA-C-N	8.71	128.34	118.85
5	U	117	SER	C-N-CA	8.71	128.34	118.85
4	L	34	ASN	N-CA-C	8.66	120.69	108.74
3	H	12	VAL	N-CA-C	8.50	119.57	108.35
1	A	115	VAL	CB-CA-C	-8.44	100.56	111.53
3	H	66	ARG	N-CA-C	-8.34	103.01	113.01
5	U	77	ASN	N-CA-C	8.31	122.84	112.87
5	U	28	ILE	N-CA-C	8.30	120.74	108.45
5	U	251	HIS	N-CA-C	-8.03	103.49	113.28
1	A	44	ILE	N-CA-C	7.72	118.54	108.35
5	U	41	VAL	CB-CA-C	-7.54	99.47	110.63
1	A	86	ALA	N-CA-C	7.40	121.89	113.02
5	U	236	TYR	N-CA-C	7.09	121.08	109.24
5	U	40	LEU	N-CA-C	7.07	121.08	109.06
4	L	115	VAL	N-CA-C	7.00	118.68	108.53
4	L	132	VAL	N-CA-C	6.97	118.33	108.36
3	H	33	TYR	CA-CB-CG	6.89	126.31	113.90
3	H	49	GLY	N-CA-C	6.82	120.09	110.74
3	H	18	VAL	N-CA-C	6.80	119.95	108.86
1	A	112	TRP	N-CA-C	6.79	117.46	107.88
1	A	123	VAL	CB-CA-C	-6.78	102.28	111.63
5	U	153	CYS	CA-C-N	-6.77	112.69	119.93
5	U	153	CYS	C-N-CA	-6.77	112.69	119.93
4	L	31	THR	N-CA-C	6.72	119.36	108.34
1	A	33	CYS	CA-C-N	6.62	128.11	119.84
1	A	33	CYS	C-N-CA	6.62	128.11	119.84
1	A	16	GLY	N-CA-C	-6.59	106.22	115.32
4	L	166	GLN	N-CA-C	-6.50	100.68	110.24
3	H	32	TYR	N-CA-C	6.45	119.78	108.75
1	A	10	ASN	N-CA-C	6.40	118.59	108.79
3	H	183	VAL	CA-C-N	6.40	126.42	119.89
3	H	183	VAL	C-N-CA	6.40	126.42	119.89
3	H	111	VAL	CB-CA-C	-6.38	99.70	111.18
3	H	30	THR	N-CA-C	-6.32	105.28	112.87
3	H	7	SER	N-CA-C	-6.18	102.37	110.53
5	U	199	GLY	N-CA-C	6.16	119.59	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	88	CYS	N-CA-C	6.14	118.42	108.41
4	L	118	PHE	CA-C-N	6.13	126.70	120.38
4	L	118	PHE	C-N-CA	6.13	126.70	120.38
5	U	225	ALA	N-CA-C	6.13	118.39	109.07
3	H	71	VAL	N-CA-C	6.09	116.93	108.23
3	H	25	SER	N-CA-C	-6.07	100.10	109.14
1	A	14	LEU	N-CA-C	6.06	118.42	109.69
3	H	142	VAL	CB-CA-C	-6.04	103.58	111.25
4	L	181	LEU	N-CA-C	6.04	117.42	108.60
4	L	17	GLN	N-CA-C	6.03	118.30	110.40
1	A	104	ASN	CA-C-N	-5.92	112.44	119.84
1	A	104	ASN	C-N-CA	-5.92	112.44	119.84
3	H	136	VAL	N-CA-C	5.89	116.84	108.42
4	L	132	VAL	CB-CA-C	-5.76	103.00	110.84
3	H	52	ASN	C-N-CD	-5.75	107.94	120.60
5	U	211	PHE	N-CA-C	5.75	117.58	108.79
4	L	86	TYR	N-CA-C	5.72	118.03	108.02
4	L	196	ALA	N-CA-C	5.72	115.39	107.73
5	U	157	ASN	N-CA-C	5.71	116.92	107.73
3	H	35	HIS	N-CA-C	5.70	117.90	109.69
3	H	150	VAL	N-CA-C	5.67	115.32	108.06
4	L	182	THR	N-CA-C	5.64	117.18	110.19
5	U	125	VAL	CB-CA-C	-5.61	102.09	111.29
1	A	57	PHE	CB-CA-C	5.58	117.98	109.34
5	U	54	THR	CB-CA-C	-5.57	103.79	112.31
5	U	272	ASN	N-CA-C	5.56	118.27	111.82
5	U	41	VAL	N-CA-C	5.53	115.85	108.11
3	H	68	THR	CA-C-N	-5.47	112.83	121.86
3	H	68	THR	C-N-CA	-5.47	112.83	121.86
5	U	17	CYS	N-CA-C	-5.45	104.71	111.90
2	B	36	THR	N-CA-C	-5.41	104.78	111.33
3	H	96	ILE	CA-C-N	5.39	131.40	121.70
3	H	96	ILE	C-N-CA	5.39	131.40	121.70
3	H	82(C)	LEU	N-CA-C	5.33	118.27	109.85
5	U	269	SER	N-CA-C	-5.33	103.59	110.19
3	H	8	GLY	CA-C-N	5.31	125.29	120.03
3	H	8	GLY	C-N-CA	5.31	125.29	120.03
1	A	74	TRP	N-CA-C	-5.29	104.97	111.75
4	L	43	SER	CA-C-N	5.29	125.58	119.92
4	L	43	SER	C-N-CA	5.29	125.58	119.92
5	U	210	THR	N-CA-C	-5.27	102.81	110.24
3	H	68	THR	CB-CA-C	-5.26	102.68	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	THR	N-CA-C	-5.25	99.61	110.80
1	A	120	LYS	CA-C-N	5.25	125.24	119.89
1	A	120	LYS	C-N-CA	5.25	125.24	119.89
3	H	118	PRO	O-C-N	5.21	123.60	121.15
5	U	11	ASP	N-CA-C	-5.20	102.21	109.96
4	L	184	ASP	N-CA-C	-5.17	104.90	111.11
5	U	194	CYS	N-CA-C	5.17	114.96	108.45
1	A	25	PHE	N-CA-C	5.16	116.72	107.80
3	H	143	LYS	N-CA-C	5.14	117.07	108.99
3	H	138	LEU	N-CA-C	5.13	117.00	108.02
3	H	177	LEU	N-CA-C	5.11	116.43	109.18
3	H	180	SER	N-CA-C	5.11	117.01	108.99
5	U	60	GLY	N-CA-C	-5.10	104.78	112.84
5	U	14	VAL	N-CA-C	5.09	116.19	108.96
5	U	243	THR	N-CA-C	5.08	117.61	110.14
3	H	206	VAL	N-CA-C	5.07	116.30	108.44
1	A	76	SER	N-CA-C	5.07	117.25	110.35
5	U	74	ASP	N-CA-C	-5.07	102.79	110.24
5	U	205	CYS	N-CA-C	5.03	119.37	112.88
3	H	20	ILE	CB-CA-C	-5.03	103.63	110.77
1	A	86	ALA	CA-C-N	-5.03	115.33	122.77
1	A	86	ALA	C-N-CA	-5.03	115.33	122.77
1	A	56	HIS	N-CA-C	-5.02	105.32	111.75
5	U	259	ASN	N-CA-C	5.01	117.07	108.90
3	H	24	ALA	N-CA-C	5.01	116.86	108.99

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	ARG	Peptide
2	B	10	THR	Peptide
3	H	51	ILE	Peptide
5	U	230	GLU	Peptide
5	U	37	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	987	0	919	336	1
2	B	312	0	272	102	0
3	H	1606	0	1560	604	1
4	L	1690	0	1649	472	0
5	U	2095	0	1946	546	0
6	C	28	0	24	3	0
6	D	28	0	25	12	0
7	U	11	0	10	3	0
8	U	14	0	13	1	0
All	All	6771	0	6418	1924	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 146.

All (1924) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	1.36	1.60
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	1.53	1.44
3:H:145:TYR:CE2	3:H:175:TYR:HB2	1.53	1.43
3:H:188:TRP:CD1	3:H:189:PRO:HA	1.52	1.43
5:U:38:LEU:HD12	5:U:39:GLU:N	1.42	1.35
5:U:39:GLU:C	5:U:40:LEU:HD22	1.48	1.34
3:H:47:TRP:NE1	4:L:96:LEU:HD13	1.44	1.33
3:H:47:TRP:CH2	3:H:49:GLY:HA2	1.67	1.28
4:L:35:TRP:CD1	4:L:48:ILE:HD12	1.68	1.28
1:A:56:HIS:HB3	1:A:57:PHE:CD1	1.68	1.28
4:L:118:PHE:O	4:L:132:VAL:HG22	1.34	1.25
4:L:35:TRP:CE3	4:L:88:CYS:HB3	1.71	1.25
3:H:154:TRP:CE3	3:H:195:CYS:HB3	1.72	1.24
5:U:203:HIS:NE2	6:D:1:NAG:O5	1.68	1.23
3:H:188:TRP:CD1	3:H:189:PRO:CA	2.23	1.22
4:L:139:PHE:CE2	4:L:144:ILE:HD12	1.75	1.21
3:H:97:TYR:O	3:H:99:HIS:CD2	1.93	1.21
3:H:32:TYR:HB3	3:H:96:ILE:CD1	1.69	1.20
5:U:27:THR:C	5:U:28:ILE:HD12	1.67	1.20
1:A:28:ILE:HD12	1:A:29:HIS:N	1.57	1.19
3:H:137:THR:HG22	3:H:182:THR:CG2	1.70	1.19
3:H:58:SER:O	3:H:59:TYR:HD1	1.20	1.18
3:H:32:TYR:CB	3:H:96:ILE:HD13	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:152:VAL:HG22	3:H:197:VAL:CG2	1.73	1.18
5:U:133:GLY:H	5:U:137:ARG:HG2	1.07	1.18
4:L:35:TRP:CZ3	4:L:88:CYS:CB	2.28	1.17
3:H:145:TYR:CE1	3:H:150:VAL:HB	1.80	1.17
5:U:31:LEU:HD22	5:U:31:LEU:N	1.58	1.17
3:H:33:TYR:O	3:H:96:ILE:HD11	1.45	1.16
3:H:83:THR:N	3:H:86:ASP:OD2	1.77	1.15
3:H:188:TRP:HD1	3:H:189:PRO:CA	1.59	1.15
5:U:71:CYS:HB2	5:U:73:LEU:CD2	1.77	1.15
1:A:40:GLN:HE22	5:U:8:THR:HG21	1.09	1.14
5:U:27:THR:O	5:U:28:ILE:HD12	1.43	1.14
5:U:203:HIS:HE2	6:D:1:NAG:C5	1.61	1.14
3:H:170:LEU:HD12	3:H:171:GLN:H	1.01	1.14
3:H:51:ILE:CG2	3:H:69:PHE:HD1	1.60	1.14
3:H:154:TRP:CZ3	3:H:195:CYS:CB	2.29	1.14
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.29	1.14
3:H:163:VAL:HG22	3:H:181:VAL:CG2	1.76	1.14
4:L:120:PRO:HB2	4:L:125:LEU:HD21	1.24	1.14
5:U:130:ILE:HG23	5:U:131:GLN:H	1.06	1.14
1:A:99:HIS:HD2	1:A:101:TYR:N	1.44	1.13
1:A:130:ASP:OD1	1:A:131:CYS:N	1.80	1.13
5:U:203:HIS:CD2	6:D:1:NAG:O6	2.00	1.13
3:H:145:TYR:HE2	3:H:175:TYR:CB	1.60	1.13
3:H:152:VAL:HG22	3:H:197:VAL:HG23	1.26	1.12
5:U:174:THR:HG22	5:U:175:LYS:HG2	1.30	1.12
1:A:28:ILE:HD12	1:A:29:HIS:H	0.95	1.12
1:A:44:ILE:CG2	1:A:60:GLY:H	1.62	1.12
3:H:66:ARG:NH1	3:H:82(B):SER:O	1.83	1.11
3:H:199:HIS:CE1	3:H:201:ALA:HB3	1.85	1.11
1:A:72:LEU:HD21	1:A:116:GLN:H	1.10	1.11
3:H:48:ILE:HD13	3:H:63:ILE:HD11	1.20	1.10
3:H:95:SER:H	3:H:96:ILE:CD1	1.63	1.10
3:H:170:LEU:HD12	3:H:171:GLN:N	1.67	1.10
3:H:145:TYR:HE1	3:H:150:VAL:CB	1.65	1.10
3:H:144:GLY:HA2	3:H:174:LEU:HD13	1.25	1.10
1:A:73:PRO:HD2	1:A:76:SER:HB3	1.18	1.10
4:L:38:GLN:HG3	4:L:44:PRO:HG3	1.23	1.10
5:U:73:LEU:HD11	5:U:76:CYS:HB3	1.11	1.10
5:U:199:GLY:HA3	5:U:204:GLY:HA3	1.33	1.10
3:H:63:ILE:HG22	3:H:65:GLY:N	1.67	1.09
4:L:142:LYS:HD3	4:L:142:LYS:H	1.15	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:148:TRP:CD2	4:L:179:LEU:HD22	1.87	1.09
1:A:115:VAL:HG21	1:A:124:GLN:HB2	1.27	1.09
3:H:97:TYR:CE2	5:U:212:LEU:HD21	1.87	1.09
5:U:43:LYS:HB3	5:U:77:ASN:HD22	0.93	1.09
2:B:27:TYR:CD1	5:U:63:ILE:HD13	1.88	1.09
1:A:40:GLN:NE2	5:U:8:THR:HG21	1.67	1.08
1:A:85:HIS:CD2	1:A:87:HIS:H	1.69	1.08
3:H:18:VAL:HG12	3:H:82(C):LEU:HD21	1.27	1.08
3:H:63:ILE:HG22	3:H:65:GLY:H	1.13	1.08
4:L:116:SER:O	4:L:117:ILE:HD13	1.53	1.08
3:H:95:SER:HB3	3:H:96:ILE:HG13	1.17	1.07
3:H:95:SER:CB	3:H:96:ILE:HG13	1.83	1.07
4:L:195:GLU:HB3	4:L:206:VAL:HG22	1.35	1.07
1:A:44:ILE:CG2	1:A:103:ARG:HH22	1.67	1.07
3:H:32:TYR:HA	3:H:96:ILE:HG21	1.09	1.07
3:H:93:ALA:HB3	3:H:100(B):LEU:HD23	1.18	1.07
5:U:203:HIS:NE2	6:D:1:NAG:C5	2.16	1.07
4:L:14:THR:HG23	4:L:107:LYS:HE3	1.14	1.06
3:H:33:TYR:H	3:H:96:ILE:HG12	1.08	1.06
5:U:71:CYS:HB2	5:U:73:LEU:HD21	1.29	1.06
3:H:188:TRP:HZ2	3:H:212:PRO:HG3	1.15	1.06
3:H:192:THR:CB	3:H:209:LYS:HE3	1.85	1.05
1:A:51:TYR:CE2	1:A:130:ASP:HB2	1.92	1.05
4:L:35:TRP:HD1	4:L:48:ILE:HD12	1.02	1.05
2:B:27:TYR:CE2	5:U:116:ARG:HD2	1.91	1.05
4:L:7:THR:HG23	4:L:8:PRO:HA	1.33	1.05
3:H:33:TYR:N	3:H:96:ILE:HG12	1.70	1.05
5:U:29:VAL:HG13	5:U:66:LEU:CD2	1.85	1.05
3:H:163:VAL:HG13	3:H:181:VAL:HB	1.07	1.04
4:L:133:VAL:HG11	4:L:135:PHE:CE2	1.92	1.04
3:H:58:SER:O	3:H:59:TYR:CD1	2.11	1.04
3:H:96:ILE:HG23	3:H:97:TYR:HA	1.35	1.04
5:U:99:GLY:H	5:U:104:SER:HB3	1.19	1.04
5:U:203:HIS:NE2	6:D:1:NAG:C6	2.21	1.04
1:A:56:HIS:O	1:A:59:ARG:NH2	1.90	1.03
3:H:18:VAL:CG1	3:H:82(C):LEU:HD21	1.88	1.03
3:H:99:HIS:O	3:H:100(A):VAL:HG13	1.57	1.03
4:L:50:LEU:HD13	4:L:53:LYS:HG3	1.04	1.03
4:L:190:ASN:OD1	4:L:211:ARG:HB2	1.57	1.03
4:L:195:GLU:CB	4:L:206:VAL:HG22	1.88	1.03
5:U:203:HIS:CD2	6:D:1:NAG:C6	2.42	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:47:TRP:CD1	4:L:96:LEU:HD13	1.93	1.03
3:H:137:THR:HG22	3:H:182:THR:HG22	1.05	1.03
3:H:47:TRP:CZ3	3:H:49:GLY:HA2	1.94	1.02
3:H:152:VAL:CG2	3:H:197:VAL:HG23	1.89	1.02
1:A:99:HIS:CD2	1:A:101:TYR:H	1.76	1.02
3:H:32:TYR:CA	3:H:96:ILE:HG21	1.89	1.02
5:U:38:LEU:HD12	5:U:39:GLU:H	0.95	1.02
1:A:72:LEU:HD23	1:A:72:LEU:H	1.24	1.02
4:L:34:ASN:HB3	4:L:49:TYR:HA	1.39	1.02
2:B:20:GLN:OE1	2:B:20:GLN:N	1.90	1.01
3:H:45:LEU:HB3	4:L:98:PHE:CD1	1.95	1.01
3:H:77:THR:HG21	3:H:79:TYR:CE1	1.95	1.01
3:H:192:THR:HB	3:H:209:LYS:CE	1.90	1.01
4:L:37:LEU:HD21	4:L:39:ARG:HG3	1.38	1.01
4:L:191:SER:HB2	4:L:210:ASN:ND2	1.74	1.01
3:H:51:ILE:CG2	3:H:69:PHE:CD1	2.44	1.01
3:H:83:THR:HG22	3:H:84:SER:N	1.74	1.01
5:U:73:LEU:CD1	5:U:76:CYS:HB3	1.90	1.01
3:H:145:TYR:HE1	3:H:150:VAL:HB	0.90	1.00
1:A:72:LEU:HD21	1:A:116:GLN:N	1.76	1.00
4:L:23:CYS:HB2	4:L:35:TRP:HH2	1.26	1.00
4:L:191:SER:HB2	4:L:210:ASN:HD21	1.26	1.00
5:U:184:LEU:O	5:U:187:LEU:N	1.93	1.00
4:L:150:ILE:HD12	4:L:155:ARG:NH1	1.77	1.00
5:U:229:HIS:CG	5:U:230:GLU:H	1.79	1.00
3:H:95:SER:H	3:H:96:ILE:CG1	1.75	1.00
2:B:13:PHE:HD1	2:B:20:GLN:HB3	1.25	0.99
3:H:51:ILE:HG22	3:H:69:PHE:CD1	1.97	0.99
5:U:219:MET:H	5:U:219:MET:CE	1.75	0.99
1:A:44:ILE:HG21	1:A:103:ARG:HH22	1.23	0.99
5:U:30:ARG:HB3	5:U:65:SER:HB3	1.45	0.99
5:U:31:LEU:HD22	5:U:31:LEU:H	1.17	0.99
5:U:239:ARG:NH2	5:U:274:PRO:HA	1.75	0.99
1:A:51:TYR:HE2	1:A:130:ASP:CA	1.74	0.99
3:H:140:CYS:HB3	3:H:179:SER:OG	1.62	0.99
5:U:168:LEU:HD22	5:U:169:LYS:N	1.78	0.99
3:H:20:ILE:O	3:H:20:ILE:HG12	1.62	0.98
3:H:145:TYR:CE2	3:H:175:TYR:CB	2.41	0.98
3:H:93:ALA:HB3	3:H:100(B):LEU:CD2	1.93	0.98
4:L:50:LEU:CD1	4:L:53:LYS:HG3	1.92	0.98
3:H:122:TYR:CE2	4:L:124:GLN:HG3	1.99	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:192:THR:HB	3:H:209:LYS:HE3	0.99	0.98
1:A:61:LYS:HA	1:A:101:TYR:CG	1.98	0.98
5:U:117:SER:OG	5:U:118:PRO:HD2	1.64	0.98
5:U:168:LEU:HD22	5:U:169:LYS:H	1.29	0.98
1:A:71:CYS:O	1:A:100:ASN:HB2	1.64	0.98
4:L:14:THR:CG2	4:L:107:LYS:HB2	1.94	0.98
4:L:116:SER:HB2	4:L:118:PHE:CE1	1.98	0.97
1:A:51:TYR:HE2	1:A:130:ASP:CB	1.77	0.97
5:U:38:LEU:CD1	5:U:39:GLU:H	1.78	0.97
3:H:154:TRP:HZ3	3:H:195:CYS:HB3	1.23	0.97
5:U:43:LYS:HB3	5:U:77:ASN:ND2	1.78	0.97
1:A:115:VAL:CG2	1:A:124:GLN:HB2	1.92	0.97
4:L:139:PHE:CD2	4:L:144:ILE:HD12	2.00	0.96
3:H:188:TRP:CZ2	3:H:212:PRO:HG3	1.99	0.96
4:L:117:ILE:C	4:L:118:PHE:HD1	1.74	0.96
3:H:163:VAL:HG22	3:H:181:VAL:HG21	1.44	0.96
5:U:239:ARG:HH22	5:U:274:PRO:HA	1.24	0.95
4:L:50:LEU:HD13	4:L:53:LYS:CG	1.97	0.95
1:A:76:SER:OG	1:A:79:VAL:HG23	1.65	0.95
3:H:163:VAL:CG1	3:H:181:VAL:HB	1.95	0.95
4:L:180:THR:C	4:L:181:LEU:HG	1.86	0.95
3:H:13:LYS:NZ	3:H:113:SER:O	1.99	0.95
5:U:71:CYS:CB	5:U:73:LEU:HD21	1.96	0.95
5:U:25:ARG:HG2	5:U:46:THR:HB	1.48	0.95
1:A:73:PRO:CD	1:A:76:SER:HB3	1.97	0.95
5:U:184:LEU:O	5:U:186:ASN:N	1.98	0.94
1:A:61:LYS:HB3	1:A:101:TYR:CE1	2.02	0.94
1:A:79:VAL:O	1:A:82:GLN:N	1.98	0.94
3:H:144:GLY:CA	3:H:174:LEU:HD13	1.96	0.94
5:U:122:CYS:O	5:U:170:CYS:HA	1.66	0.94
4:L:14:THR:O	4:L:17:GLN:HB2	1.68	0.94
5:U:38:LEU:CD1	5:U:39:GLU:N	2.31	0.94
2:B:25:CYS:SG	2:B:26:SER:N	2.39	0.94
4:L:14:THR:HG23	4:L:107:LYS:HB2	1.49	0.94
1:A:58:TYR:OH	1:A:61:LYS:O	1.85	0.94
3:H:32:TYR:HD2	3:H:96:ILE:HB	1.30	0.94
3:H:51:ILE:HG22	3:H:69:PHE:HD1	1.29	0.94
3:H:95:SER:HB3	3:H:96:ILE:CG1	1.98	0.94
5:U:208:GLU:N	5:U:208:GLU:OE1	2.01	0.94
1:A:56:HIS:HB3	1:A:57:PHE:HD1	1.13	0.94
1:A:92:LEU:HD23	1:A:92:LEU:H	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:53:TYR:HE2	5:U:214:ASP:OD2	1.51	0.94
3:H:137:THR:CG2	3:H:182:THR:HG22	1.96	0.94
5:U:73:LEU:HD11	5:U:76:CYS:CB	1.97	0.94
4:L:192:TYR:HD2	4:L:209:PHE:CZ	1.85	0.94
3:H:166:PHE:CG	4:L:176:SER:HB3	2.02	0.93
3:H:166:PHE:CD1	4:L:176:SER:HB3	2.02	0.93
1:A:44:ILE:HD12	1:A:44:ILE:N	1.82	0.93
3:H:20:ILE:O	3:H:20:ILE:CG1	2.15	0.93
3:H:48:ILE:HD13	3:H:63:ILE:CD1	1.97	0.93
4:L:108:ARG:HD3	4:L:172:THR:HG23	1.51	0.93
1:A:99:HIS:CD2	1:A:101:TYR:N	2.35	0.93
1:A:51:TYR:H	1:A:51:TYR:HD2	1.12	0.93
4:L:117:ILE:HD12	4:L:134:CYS:SG	2.08	0.93
2:B:6:LYS:HE3	2:B:38:GLU:OE1	1.69	0.92
2:B:13:PHE:HD1	2:B:20:GLN:CB	1.82	0.92
4:L:14:THR:CG2	4:L:107:LYS:HE3	1.99	0.92
4:L:35:TRP:HZ3	4:L:88:CYS:HB3	1.33	0.92
1:A:51:TYR:CE2	1:A:130:ASP:HA	2.04	0.92
4:L:37:LEU:HD12	4:L:38:GLN:N	1.84	0.92
2:B:22:ASP:OD1	2:B:24:LEU:N	2.03	0.92
3:H:101:ASP:HA	4:L:46:ARG:HD3	1.49	0.92
3:H:6:GLN:CB	3:H:105:GLN:HE22	1.81	0.92
4:L:148:TRP:CE2	4:L:179:LEU:HD22	2.04	0.92
5:U:199:GLY:H	5:U:236:TYR:HE1	1.16	0.92
3:H:33:TYR:CZ	3:H:98:GLY:HA2	2.04	0.92
5:U:61:LEU:HD12	5:U:61:LEU:N	1.83	0.92
1:A:63:SER:C	1:A:64:THR:HG22	1.94	0.92
3:H:97:TYR:CE2	5:U:212:LEU:CD2	2.53	0.92
5:U:133:GLY:HA3	5:U:137:ARG:NE	1.85	0.92
5:U:246:MET:HB3	5:U:252:LEU:HD13	1.51	0.92
5:U:113:LEU:HD23	5:U:113:LEU:O	1.70	0.91
3:H:199:HIS:HE1	3:H:201:ALA:HB3	1.29	0.91
1:A:73:PRO:HD2	1:A:76:SER:CB	2.00	0.91
3:H:37:VAL:CG1	4:L:98:PHE:HE1	1.83	0.91
3:H:83:THR:O	3:H:86:ASP:HB2	1.68	0.91
3:H:95:SER:H	3:H:96:ILE:HG13	1.34	0.91
4:L:92:THR:O	4:L:93:HIS:ND1	2.03	0.91
1:A:88:ARG:NH1	1:A:90:ASP:OD2	2.04	0.91
2:B:26:SER:O	2:B:29:GLN:N	2.03	0.91
4:L:7:THR:CG2	4:L:8:PRO:HA	2.00	0.91
4:L:33:LEU:HB3	4:L:51:VAL:CG2	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:38:LEU:HD12	5:U:38:LEU:C	1.89	0.91
3:H:143:LYS:HG3	3:H:176:THR:OG1	1.70	0.91
3:H:91:TYR:CE1	3:H:105:GLN:O	2.24	0.90
3:H:97:TYR:O	3:H:99:HIS:HD2	1.48	0.90
1:A:96:LEU:N	1:A:96:LEU:HD23	1.81	0.90
5:U:199:GLY:HA3	5:U:204:GLY:CA	2.01	0.90
4:L:139:PHE:CE2	4:L:144:ILE:CD1	2.54	0.90
4:L:8:PRO:CG	4:L:11:LEU:HD22	2.01	0.90
4:L:9:LEU:H	4:L:9:LEU:HD12	1.35	0.90
1:A:87:HIS:CE1	5:U:11:ASP:HA	2.07	0.90
4:L:108:ARG:HD3	4:L:172:THR:CG2	2.00	0.90
4:L:38:GLN:HG3	4:L:44:PRO:CG	2.01	0.89
1:A:25:PHE:N	1:A:25:PHE:CD1	2.36	0.89
3:H:154:TRP:CD1	3:H:163:VAL:HG11	2.08	0.89
2:B:27:TYR:HD1	5:U:63:ILE:HD13	1.36	0.89
3:H:32:TYR:HB3	3:H:96:ILE:HD13	0.90	0.89
1:A:51:TYR:HE2	1:A:130:ASP:HA	1.34	0.89
4:L:120:PRO:HB2	4:L:125:LEU:CD2	2.01	0.89
4:L:148:TRP:CG	4:L:179:LEU:HD22	2.06	0.89
5:U:219:MET:HB3	5:U:242:ALA:CA	2.02	0.89
5:U:195:TYR:HB2	5:U:272:ASN:HB3	1.54	0.89
5:U:16:GLU:H	5:U:16:GLU:CD	1.74	0.89
5:U:98:CYS:O	5:U:105:CYS:SG	2.31	0.89
3:H:33:TYR:CE2	3:H:52:ASN:ND2	2.39	0.89
3:H:118:PRO:HA	3:H:199:HIS:CD2	2.07	0.89
5:U:130:ILE:HG23	5:U:131:GLN:N	1.88	0.89
3:H:21:SER:HB2	3:H:23:LYS:NZ	1.87	0.89
3:H:31:SER:HA	5:U:212:LEU:HD13	1.53	0.89
1:A:85:HIS:HD2	1:A:87:HIS:H	1.20	0.89
3:H:114:ALA:HB3	3:H:146:PHE:HE1	1.34	0.88
5:U:4:MET:HE2	5:U:78:GLN:CB	2.02	0.88
3:H:32:TYR:HA	3:H:96:ILE:CG2	2.02	0.88
1:A:13:CYS:SG	1:A:19:CYS:HB2	2.12	0.88
3:H:136:VAL:HG22	3:H:183:VAL:O	1.72	0.88
3:H:95:SER:N	3:H:96:ILE:HG13	1.89	0.88
3:H:188:TRP:HA	3:H:190:SER:H	1.36	0.88
3:H:146:PHE:CB	3:H:174:LEU:HD23	2.03	0.88
3:H:180:SER:HB3	4:L:135:PHE:CE1	2.06	0.88
5:U:97:SER:HA	5:U:145:ARG:O	1.73	0.88
1:A:93:GLN:O	1:A:94:LEU:HD23	1.73	0.88
3:H:126:PRO:HD2	3:H:188:TRP:HH2	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:45:LEU:HB3	4:L:98:PHE:HD1	1.35	0.88
1:A:13:CYS:C	1:A:14:LEU:HD22	1.99	0.88
3:H:140:CYS:HB2	3:H:154:TRP:HH2	1.38	0.87
4:L:116:SER:HB2	4:L:118:PHE:HE1	1.37	0.87
4:L:140:TYR:HB2	4:L:172:THR:HG22	1.56	0.87
3:H:112:SER:OG	3:H:113:SER:N	2.00	0.87
3:H:119:PRO:HD3	3:H:199:HIS:HD2	1.39	0.87
3:H:18:VAL:HG12	3:H:82(C):LEU:CD2	2.03	0.87
1:A:88:ARG:O	1:A:89:SER:C	2.16	0.87
1:A:56:HIS:HB3	1:A:57:PHE:CE1	2.09	0.87
3:H:93:ALA:CB	3:H:100(B):LEU:HD23	2.04	0.87
5:U:23:LEU:HD13	5:U:70:VAL:HG21	1.55	0.87
3:H:94:ARG:HB3	3:H:96:ILE:HD12	1.53	0.87
3:H:152:VAL:HG13	3:H:197:VAL:HG23	1.55	0.87
3:H:146:PHE:HB3	3:H:174:LEU:HD23	1.57	0.87
4:L:90:GLN:NE2	4:L:97:THR:OG1	2.08	0.87
4:L:186:TYR:CE1	4:L:192:TYR:HE2	1.93	0.87
5:U:133:GLY:H	5:U:137:ARG:CG	1.86	0.87
5:U:134:GLU:OE2	5:U:135:GLU:HG3	1.74	0.87
2:B:7:GLY:C	2:B:9:CYS:H	1.80	0.87
1:A:73:PRO:HA	1:A:100:ASN:HA	1.57	0.86
5:U:129:TRP:NE1	5:U:138:PRO:HG2	1.90	0.86
5:U:273:HIS:CG	5:U:274:PRO:HD2	2.09	0.86
4:L:142:LYS:HD3	4:L:142:LYS:N	1.90	0.86
1:A:69:ARG:HB2	1:A:70:PRO:HD2	1.55	0.86
3:H:117:THR:N	3:H:146:PHE:O	2.09	0.86
1:A:28:ILE:CD1	1:A:29:HIS:N	2.38	0.86
3:H:119:PRO:CB	3:H:145:TYR:HB3	2.04	0.86
4:L:23:CYS:HB2	4:L:35:TRP:CH2	2.09	0.86
4:L:23:CYS:C	4:L:24:LYS:HD2	2.00	0.86
3:H:33:TYR:CE2	3:H:98:GLY:N	2.43	0.86
4:L:38:GLN:CG	4:L:44:PRO:HG3	2.04	0.86
3:H:47:TRP:CD1	4:L:96:LEU:HB2	2.10	0.86
3:H:47:TRP:CE2	4:L:96:LEU:HD13	2.11	0.86
5:U:23:LEU:HB2	5:U:46:THR:O	1.75	0.86
5:U:54:THR:HG21	5:U:120:GLU:OE1	1.75	0.86
1:A:25:PHE:N	1:A:25:PHE:HD1	1.74	0.85
4:L:186:TYR:HE1	4:L:192:TYR:HE2	1.23	0.85
5:U:199:GLY:CA	5:U:204:GLY:HA3	2.06	0.85
5:U:219:MET:H	5:U:219:MET:HE2	1.41	0.85
3:H:2:VAL:HG11	3:H:102:TYR:CD2	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TYR:C	2:B:27:TYR:CD2	2.54	0.85
5:U:195:TYR:O	5:U:272:ASN:ND2	2.10	0.85
1:A:14:LEU:HD22	1:A:14:LEU:N	1.92	0.85
3:H:37:VAL:HG21	3:H:103:TRP:CZ3	2.11	0.85
3:H:47:TRP:CH2	3:H:49:GLY:CA	2.55	0.85
4:L:156:GLN:OE1	4:L:156:GLN:N	2.08	0.85
2:B:2:GLN:N	2:B:18:LYS:HZ2	1.75	0.85
5:U:130:ILE:CG2	5:U:131:GLN:H	1.90	0.85
4:L:27(C):LEU:HD12	4:L:31:THR:OG1	1.77	0.85
5:U:219:MET:HB3	5:U:242:ALA:HA	1.57	0.84
1:A:15:ASN:ND2	1:A:37:PHE:CE1	2.45	0.84
4:L:82:ASP:O	4:L:104:LEU:HD23	1.78	0.84
1:A:51:TYR:HE2	1:A:130:ASP:HB2	1.32	0.84
3:H:21:SER:HB2	3:H:23:LYS:HZ1	1.39	0.84
3:H:51:ILE:HG21	3:H:69:PHE:HD1	1.42	0.84
3:H:95:SER:CA	3:H:96:ILE:HG13	2.07	0.84
3:H:163:VAL:HG22	3:H:181:VAL:HG23	1.58	0.84
4:L:14:THR:HG23	4:L:107:LYS:CE	2.05	0.84
1:A:44:ILE:CG2	1:A:60:GLY:N	2.41	0.84
1:A:93:GLN:C	1:A:94:LEU:HD23	2.02	0.84
2:B:27:TYR:CD2	2:B:27:TYR:O	2.29	0.84
3:H:32:TYR:CD2	3:H:96:ILE:HB	2.11	0.84
4:L:118:PHE:O	4:L:132:VAL:CG2	2.23	0.84
1:A:99:HIS:HD2	1:A:101:TYR:H	0.85	0.84
3:H:4:LEU:HD23	3:H:23:LYS:O	1.76	0.84
4:L:35:TRP:HD1	4:L:48:ILE:CD1	1.88	0.84
5:U:203:HIS:CE1	6:D:1:NAG:O5	2.31	0.84
3:H:152:VAL:CG1	3:H:197:VAL:HG23	2.08	0.83
4:L:116:SER:CB	4:L:118:PHE:HE1	1.90	0.83
5:U:39:GLU:C	5:U:40:LEU:CD2	2.44	0.83
5:U:99:GLY:O	5:U:104:SER:N	2.12	0.83
1:A:44:ILE:CG2	1:A:103:ARG:NH2	2.42	0.83
5:U:126:VAL:HG22	5:U:143:HIS:CD2	2.13	0.83
5:U:157:ASN:HB2	5:U:245:SER:OG	1.78	0.83
3:H:45:LEU:HD12	4:L:87:TYR:CE2	2.14	0.83
3:H:77:THR:CG2	3:H:79:TYR:CE1	2.62	0.83
3:H:83:THR:CG2	3:H:84:SER:N	2.42	0.83
3:H:188:TRP:HD1	3:H:189:PRO:HA	0.71	0.83
4:L:185:GLU:OE1	4:L:188:ARG:HD3	1.79	0.83
2:B:7:GLY:O	2:B:9:CYS:N	2.12	0.82
3:H:83:THR:HG22	3:H:84:SER:H	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:CD1	2:B:20:GLN:HB3	2.12	0.82
4:L:17:GLN:O	4:L:78:VAL:HG23	1.79	0.82
1:A:41:HIS:ND1	1:A:92:LEU:HD11	1.94	0.82
3:H:154:TRP:CE3	3:H:195:CYS:CB	2.59	0.82
3:H:119:PRO:HD3	3:H:199:HIS:CD2	2.14	0.82
5:U:190:ASN:ND2	5:U:215:CYS:HB2	1.94	0.82
1:A:69:ARG:CB	1:A:70:PRO:HD2	2.10	0.81
3:H:95:SER:OG	3:H:96:ILE:HA	1.79	0.81
3:H:6:GLN:HB2	3:H:105:GLN:NE2	1.95	0.81
3:H:51:ILE:HG21	3:H:69:PHE:CD1	2.14	0.81
5:U:187:LEU:HD23	5:U:217:GLY:HA3	1.62	0.81
1:A:104:ASN:HB2	1:A:111:PRO:HA	1.63	0.81
2:B:27:TYR:CE2	5:U:116:ARG:CD	2.63	0.81
2:B:13:PHE:CD1	2:B:20:GLN:HG3	2.15	0.81
3:H:95:SER:N	3:H:96:ILE:CD1	2.41	0.81
5:U:216:ARG:HG2	5:U:216:ARG:HH11	1.44	0.81
1:A:84:TYR:HD2	1:A:88:ARG:NH2	1.78	0.81
5:U:203:HIS:CD2	6:D:1:NAG:H61	2.13	0.81
1:A:85:HIS:CD2	1:A:87:HIS:N	2.47	0.81
3:H:83:THR:CG2	3:H:84:SER:H	1.94	0.81
3:H:39:GLN:O	3:H:88:ALA:HB1	1.81	0.81
1:A:59:ARG:HA	1:A:103:ARG:CZ	2.10	0.80
2:B:34:ASP:O	2:B:37:ALA:HB3	1.80	0.80
3:H:91:TYR:HE1	3:H:105:GLN:O	1.64	0.80
5:U:98:CYS:C	5:U:105:CYS:SG	2.64	0.80
1:A:51:TYR:CE2	1:A:130:ASP:CB	2.60	0.80
1:A:115:VAL:HG21	1:A:124:GLN:CB	2.09	0.80
3:H:124:LEU:HD11	3:H:141:LEU:HD22	1.63	0.80
3:H:210:ILE:HG22	3:H:212:PRO:HD3	1.61	0.80
3:H:33:TYR:H	3:H:96:ILE:CG1	1.93	0.80
3:H:48:ILE:CD1	3:H:63:ILE:HD11	2.08	0.80
4:L:46:ARG:CZ	4:L:49:TYR:HE1	1.94	0.80
5:U:190:ASN:HD21	5:U:215:CYS:CB	1.95	0.80
3:H:37:VAL:CG1	4:L:98:PHE:CE1	2.65	0.80
1:A:15:ASN:CG	1:A:37:PHE:CE1	2.60	0.80
3:H:59:TYR:OH	3:H:68:THR:HA	1.82	0.80
4:L:192:TYR:HB2	4:L:209:PHE:CE2	2.16	0.80
4:L:1:ASP:OD2	4:L:95:PRO:HG2	1.80	0.80
5:U:4:MET:HE2	5:U:78:GLN:HB3	1.64	0.80
4:L:151:ASP:OD2	4:L:189:HIS:HB3	1.81	0.79
5:U:43:LYS:CB	5:U:77:ASN:HD22	1.86	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:149:PRO:HG2	3:H:200:PRO:HD2	1.64	0.79
3:H:154:TRP:HD1	3:H:163:VAL:HG11	1.48	0.79
4:L:106:LEU:HD22	4:L:106:LEU:N	1.96	0.79
4:L:133:VAL:HG11	4:L:135:PHE:CD2	2.16	0.79
5:U:167:PHE:CD2	5:U:182:LEU:HD12	2.17	0.79
1:A:44:ILE:HG23	1:A:103:ARG:NH2	1.98	0.79
3:H:100(A):VAL:HA	4:L:89:TRP:CH2	2.18	0.79
5:U:219:MET:H	5:U:219:MET:HE3	1.47	0.79
1:A:72:LEU:HD23	1:A:114:TYR:O	1.83	0.79
4:L:1:ASP:OD2	4:L:95:PRO:CG	2.31	0.79
5:U:119:GLU:O	5:U:121:GLN:HG3	1.80	0.79
5:U:57:TYR:HE1	5:U:59:THR:HG23	1.48	0.79
3:H:116:THR:HG22	3:H:201:ALA:HB1	1.65	0.79
3:H:166:PHE:CD1	4:L:176:SER:CB	2.65	0.79
2:B:40:LYS:NZ	5:U:35:GLY:HA3	1.97	0.79
3:H:90:TYR:HB2	3:H:107:THR:HG22	1.64	0.79
3:H:69:PHE:N	3:H:69:PHE:HD2	1.81	0.79
5:U:103:MET:O	5:U:107:ARG:HG3	1.83	0.79
5:U:123:LEU:HD12	5:U:123:LEU:N	1.98	0.79
1:A:44:ILE:HG22	1:A:60:GLY:H	1.46	0.79
3:H:100(A):VAL:CG2	3:H:100(A):VAL:O	2.31	0.79
5:U:71:CYS:HB2	5:U:73:LEU:HD23	1.62	0.79
1:A:79:VAL:HG13	1:A:114:TYR:CE2	2.18	0.78
4:L:8:PRO:HG3	4:L:11:LEU:HD22	1.65	0.78
4:L:46:ARG:HH21	4:L:55:ASP:CG	1.90	0.78
1:A:44:ILE:HG22	1:A:60:GLY:N	1.98	0.78
1:A:69:ARG:CB	1:A:70:PRO:CD	2.61	0.78
3:H:97:TYR:CD2	5:U:212:LEU:HD21	2.17	0.78
3:H:123:PRO:HB3	3:H:208:LYS:HD2	1.65	0.78
3:H:138:LEU:HD13	3:H:193:VAL:HG11	1.66	0.78
4:L:27(D):ASP:OD1	4:L:28:ASP:HB3	1.83	0.78
5:U:40:LEU:HD22	5:U:40:LEU:N	1.96	0.78
3:H:118:PRO:HA	3:H:199:HIS:HD2	1.46	0.78
5:U:39:GLU:CA	5:U:40:LEU:HD22	2.14	0.78
5:U:195:TYR:HB2	5:U:272:ASN:HD22	1.47	0.78
3:H:145:TYR:O	3:H:145:TYR:CD2	2.37	0.78
4:L:46:ARG:HD2	4:L:49:TYR:HD1	1.48	0.78
4:L:139:PHE:HE2	4:L:144:ILE:HB	1.46	0.78
3:H:47:TRP:NE1	4:L:96:LEU:CD1	2.38	0.78
5:U:4:MET:HE2	5:U:78:GLN:HB2	1.65	0.78
3:H:72:ASP:HB3	3:H:75:SER:OG	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:HD22	5:U:66:LEU:CD1	1.97	0.78
3:H:37:VAL:HG11	4:L:98:PHE:HE1	1.47	0.78
4:L:117:ILE:C	4:L:118:PHE:CD1	2.60	0.78
1:A:61:LYS:HG2	1:A:101:TYR:CE2	2.19	0.77
5:U:9:ASN:C	5:U:9:ASN:OD1	2.26	0.77
1:A:123:VAL:O	1:A:124:GLN:HG2	1.85	0.77
3:H:145:TYR:CD2	3:H:175:TYR:HB2	2.18	0.77
1:A:44:ILE:HG23	1:A:103:ARG:HH22	1.50	0.77
3:H:114:ALA:HB3	3:H:146:PHE:CE1	2.19	0.77
1:A:15:ASN:ND2	1:A:37:PHE:HE1	1.81	0.77
4:L:161:ASN:HB3	4:L:175:MET:CE	2.15	0.77
5:U:123:LEU:HB3	5:U:169:LYS:O	1.85	0.77
1:A:72:LEU:HD23	1:A:72:LEU:N	2.00	0.77
3:H:145:TYR:CE1	3:H:150:VAL:CB	2.55	0.77
4:L:105:GLU:OE2	4:L:173:TYR:OH	2.02	0.77
5:U:199:GLY:N	5:U:236:TYR:HE1	1.82	0.77
3:H:43:LYS:HE2	3:H:43:LYS:HA	1.66	0.77
4:L:37:LEU:HD12	4:L:38:GLN:H	1.47	0.77
5:U:195:TYR:HD1	5:U:210:THR:HG22	1.47	0.77
5:U:16:GLU:CD	5:U:16:GLU:N	2.43	0.77
2:B:13:PHE:CD1	2:B:20:GLN:CB	2.66	0.76
5:U:219:MET:HG3	5:U:243:THR:HG23	1.67	0.76
1:A:22:ASN:HA	5:U:140:ASP:OD2	1.86	0.76
1:A:94:LEU:HD13	1:A:105:PRO:HG3	1.64	0.76
5:U:29:VAL:HG13	5:U:66:LEU:HD23	1.67	0.76
5:U:133:GLY:N	5:U:137:ARG:HG2	1.93	0.76
5:U:107:ARG:HB2	5:U:109:ARG:HH11	1.49	0.76
5:U:137:ARG:HD3	5:U:138:PRO:HD2	1.66	0.76
3:H:94:ARG:O	3:H:100(B):LEU:HA	1.86	0.76
3:H:122:TYR:CD2	4:L:124:GLN:NE2	2.54	0.76
3:H:163:VAL:HG13	3:H:181:VAL:CB	2.03	0.76
3:H:2:VAL:HG21	3:H:102:TYR:CD2	2.20	0.76
3:H:59:TYR:HE2	3:H:67:ALA:O	1.68	0.76
3:H:90:TYR:HB2	3:H:107:THR:CG2	2.16	0.76
3:H:188:TRP:HE1	3:H:212:PRO:HG2	1.49	0.76
5:U:14:VAL:CG1	5:U:15:GLU:N	2.48	0.76
5:U:137:ARG:HH22	5:U:198:LYS:NZ	1.82	0.76
4:L:124:GLN:HG2	4:L:129:GLY:O	1.86	0.76
3:H:97:TYR:HD2	5:U:212:LEU:HD11	1.48	0.76
5:U:14:VAL:HG12	5:U:15:GLU:N	1.99	0.76
2:B:27:TYR:HD1	5:U:63:ILE:CD1	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:59:TYR:CE2	3:H:67:ALA:O	2.38	0.76
2:B:26:SER:C	2:B:29:GLN:H	1.94	0.76
3:H:33:TYR:N	3:H:96:ILE:CG1	2.47	0.75
5:U:27:THR:C	5:U:28:ILE:CD1	2.55	0.75
1:A:40:GLN:HE22	5:U:8:THR:CG2	1.97	0.75
4:L:46:ARG:CZ	4:L:49:TYR:CE1	2.68	0.75
4:L:211:ARG:NH1	4:L:211:ARG:HB3	2.02	0.75
5:U:31:LEU:N	5:U:31:LEU:CD2	2.38	0.75
1:A:80:LEU:HD23	1:A:85:HIS:CD2	2.20	0.75
4:L:90:GLN:NE2	4:L:90:GLN:O	2.20	0.75
4:L:66:GLY:HA3	4:L:71:PHE:HA	1.68	0.75
4:L:192:TYR:CD2	4:L:209:PHE:CZ	2.74	0.75
5:U:31:LEU:H	5:U:31:LEU:CD2	1.95	0.75
5:U:98:CYS:SG	5:U:145:ARG:HG2	2.27	0.75
3:H:100(A):VAL:O	3:H:100(A):VAL:HG23	1.87	0.75
3:H:169:VAL:HB	3:H:176:THR:O	1.87	0.75
4:L:161:ASN:HB3	4:L:175:MET:HE1	1.66	0.75
3:H:59:TYR:CE1	3:H:69:PHE:CE2	2.75	0.74
3:H:140:CYS:HB2	3:H:154:TRP:CH2	2.22	0.74
4:L:164:THR:HB	4:L:174:SER:HB2	1.66	0.74
4:L:148:TRP:NE1	4:L:179:LEU:HD13	2.02	0.74
5:U:190:ASN:HD21	5:U:215:CYS:C	1.96	0.74
1:A:14:LEU:N	1:A:14:LEU:CD2	2.50	0.74
5:U:127:THR:O	5:U:142:ARG:HA	1.88	0.74
1:A:56:HIS:NE2	1:A:107:ASN:ND2	2.35	0.74
4:L:51:VAL:HG21	4:L:71:PHE:HE2	1.50	0.74
4:L:61:ARG:NH1	4:L:77:ARG:O	2.21	0.74
3:H:6:GLN:HB2	3:H:105:GLN:HE22	1.49	0.74
3:H:50:GLU:HG2	3:H:58:SER:OG	1.88	0.74
3:H:100(B):LEU:HD12	3:H:100(B):LEU:N	2.02	0.74
4:L:6:GLN:HG3	4:L:100:ALA:H	1.52	0.74
5:U:195:TYR:CB	5:U:272:ASN:HD22	2.00	0.74
3:H:36:TRP:CZ2	3:H:79:TYR:O	2.41	0.74
3:H:97:TYR:CD2	5:U:212:LEU:HD11	2.23	0.74
1:A:61:LYS:HB3	1:A:101:TYR:CD1	2.21	0.74
1:A:94:LEU:HD13	1:A:105:PRO:CB	2.17	0.74
3:H:95:SER:N	3:H:96:ILE:CG1	2.48	0.74
5:U:113:LEU:HD23	5:U:113:LEU:C	2.13	0.74
5:U:229:HIS:CD2	5:U:230:GLU:H	2.06	0.74
3:H:33:TYR:O	3:H:96:ILE:CD1	2.32	0.73
3:H:95:SER:CB	3:H:96:ILE:HA	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:197:VAL:HG12	3:H:206:VAL:HG12	1.70	0.73
4:L:124:GLN:OE1	4:L:131:SER:N	2.21	0.73
3:H:192:THR:HG21	3:H:209:LYS:NZ	2.03	0.73
4:L:33:LEU:HD12	4:L:51:VAL:HG22	1.70	0.73
5:U:119:GLU:CD	5:U:119:GLU:H	1.96	0.73
5:U:252:LEU:HG	5:U:256:PHE:CE1	2.23	0.73
3:H:58:SER:C	3:H:59:TYR:HD1	1.96	0.73
4:L:35:TRP:CE3	4:L:88:CYS:CB	2.61	0.73
5:U:137:ARG:HB3	5:U:138:PRO:HD2	1.70	0.73
3:H:95:SER:H	3:H:96:ILE:HD12	1.53	0.73
5:U:133:GLY:HA3	5:U:137:ARG:CZ	2.19	0.73
4:L:73:LEU:HD12	4:L:74:LYS:H	1.53	0.73
4:L:89:TRP:HB3	4:L:98:PHE:CD2	2.21	0.73
4:L:17:GLN:HB3	4:L:18:PRO:HD2	1.69	0.73
4:L:195:GLU:HB2	4:L:206:VAL:HG22	1.70	0.73
5:U:133:GLY:CA	5:U:137:ARG:CZ	2.66	0.73
1:A:34:PRO:O	1:A:35:LYS:HG2	1.89	0.73
3:H:31:SER:CA	5:U:212:LEU:HD13	2.18	0.73
3:H:37:VAL:HG11	4:L:98:PHE:CE1	2.21	0.73
5:U:32:TRP:CE3	5:U:32:TRP:C	2.66	0.73
5:U:187:LEU:HB3	5:U:188:PRO:HD2	1.70	0.73
5:U:230:GLU:HB3	5:U:231:PRO:CD	2.19	0.73
5:U:107:ARG:CB	5:U:109:ARG:HH11	2.02	0.73
5:U:153:CYS:O	5:U:154:PRO:C	2.30	0.73
1:A:85:HIS:CD2	1:A:85:HIS:C	2.67	0.72
2:B:2:GLN:OE1	2:B:4:SER:OG	2.02	0.72
1:A:63:SER:C	1:A:64:THR:CG2	2.61	0.72
5:U:229:HIS:CG	5:U:230:GLU:N	2.47	0.72
3:H:6:GLN:H	3:H:105:GLN:HE22	1.37	0.72
1:A:40:GLN:NE2	5:U:8:THR:CG2	2.52	0.72
3:H:48:ILE:CD1	3:H:63:ILE:CD1	2.67	0.72
5:U:100:SER:OG	5:U:106:GLU:OE1	2.06	0.72
5:U:195:TYR:CA	5:U:272:ASN:HD22	2.02	0.72
5:U:221:GLN:HB2	5:U:242:ALA:O	1.88	0.72
5:U:190:ASN:HD21	5:U:215:CYS:HB2	1.52	0.72
3:H:95:SER:O	3:H:100(A):VAL:O	2.08	0.72
3:H:68:THR:HG22	3:H:69:PHE:O	1.88	0.72
4:L:188:ARG:O	4:L:189:HIS:ND1	2.23	0.72
4:L:13:VAL:O	4:L:106:LEU:HA	1.88	0.72
5:U:57:TYR:CE1	5:U:59:THR:HG23	2.24	0.72
3:H:33:TYR:HB2	3:H:96:ILE:HG12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:CE1	2:B:20:GLN:HG3	2.25	0.71
3:H:4:LEU:HB3	3:H:104:GLY:CA	2.19	0.71
3:H:69:PHE:N	3:H:69:PHE:CD2	2.56	0.71
1:A:51:TYR:CE2	1:A:130:ASP:CA	2.64	0.71
1:A:51:TYR:CZ	1:A:130:ASP:HB2	2.24	0.71
3:H:29:PHE:C	3:H:31:SER:H	1.98	0.71
4:L:92:THR:C	4:L:93:HIS:HD1	1.98	0.71
2:B:13:PHE:CD1	2:B:20:GLN:CG	2.74	0.71
2:B:16:ASP:O	2:B:17:LYS:HB2	1.88	0.71
1:A:96:LEU:N	1:A:96:LEU:CD2	2.53	0.71
3:H:142:VAL:HG23	3:H:177:LEU:HD11	1.70	0.71
5:U:216:ARG:HG2	5:U:216:ARG:NH1	2.01	0.71
2:B:8:ARG:O	2:B:10:THR:N	2.21	0.71
4:L:37:LEU:HD12	4:L:85:VAL:O	1.90	0.71
4:L:148:TRP:CG	4:L:179:LEU:CD2	2.73	0.71
3:H:45:LEU:HD12	4:L:87:TYR:CD2	2.24	0.71
3:H:53:TYR:CE2	5:U:214:ASP:OD2	2.40	0.71
1:A:59:ARG:HA	1:A:103:ARG:NH1	2.05	0.71
4:L:60:ASP:N	4:L:60:ASP:OD1	2.19	0.71
4:L:180:THR:C	4:L:181:LEU:CG	2.61	0.71
5:U:129:TRP:CE2	5:U:138:PRO:HG2	2.25	0.71
3:H:95:SER:N	3:H:96:ILE:HD12	2.04	0.71
3:H:146:PHE:CD2	3:H:147:PRO:HA	2.26	0.71
3:H:170:LEU:HD22	3:H:175:TYR:CE2	2.25	0.71
4:L:59:PRO:HG2	4:L:62:PHE:HE1	1.56	0.71
4:L:14:THR:HG22	4:L:107:LYS:HB2	1.71	0.71
5:U:7:LYS:HE3	5:U:11:ASP:HB2	1.72	0.71
5:U:184:LEU:C	5:U:186:ASN:N	2.46	0.71
1:A:72:LEU:H	1:A:72:LEU:CD2	1.97	0.71
3:H:12:VAL:O	3:H:111:VAL:HG12	1.91	0.71
3:H:123:PRO:HD2	4:L:121:SER:CB	2.21	0.71
3:H:166:PHE:CZ	4:L:175:MET:C	2.69	0.71
3:H:166:PHE:CE2	4:L:175:MET:C	2.69	0.71
5:U:3:CYS:HA	5:U:75:LEU:HD23	1.72	0.71
5:U:132:GLU:HG3	5:U:136:GLY:N	2.06	0.71
4:L:9:LEU:HD12	4:L:9:LEU:N	2.06	0.70
1:A:35:LYS:HG2	1:A:36:LYS:H	1.56	0.70
4:L:37:LEU:CD1	4:L:85:VAL:O	2.39	0.70
4:L:121:SER:O	4:L:125:LEU:HD23	1.90	0.70
1:A:56:HIS:CD2	1:A:107:ASN:OD1	2.44	0.70
3:H:90:TYR:O	3:H:107:THR:HB	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:117:ILE:HG23	4:L:133:VAL:O	1.91	0.70
4:L:138:ASN:HA	4:L:173:TYR:O	1.90	0.70
4:L:142:LYS:HB3	4:L:173:TYR:CD1	2.26	0.70
5:U:193:GLN:O	5:U:269:SER:HB3	1.92	0.70
5:U:219:MET:CE	5:U:219:MET:N	2.54	0.70
4:L:33:LEU:HB3	4:L:51:VAL:HG22	1.72	0.70
5:U:90:SER:HB2	5:U:92:TYR:CZ	2.26	0.70
5:U:126:VAL:CG2	5:U:143:HIS:CD2	2.75	0.70
3:H:2:VAL:HG11	3:H:102:TYR:CB	2.21	0.70
3:H:167:PRO:HD2	4:L:162:SER:OG	1.92	0.70
4:L:148:TRP:CD1	4:L:179:LEU:HD22	2.25	0.70
3:H:88:ALA:O	3:H:109:VAL:HG23	1.92	0.70
5:U:52:ASN:OD1	5:U:69:VAL:HA	1.92	0.70
5:U:219:MET:HE2	5:U:219:MET:N	2.06	0.70
1:A:92:LEU:H	1:A:92:LEU:CD2	2.04	0.70
2:B:5:CYS:HB2	2:B:34:ASP:OD2	1.91	0.70
2:B:8:ARG:C	2:B:10:THR:H	1.99	0.70
2:B:27:TYR:HE2	5:U:116:ARG:CD	2.05	0.70
3:H:103:TRP:CZ2	4:L:36:LEU:HD22	2.27	0.70
1:A:97:GLY:C	1:A:99:HIS:H	1.99	0.69
3:H:100(A):VAL:HA	4:L:89:TRP:CZ3	2.27	0.69
1:A:94:LEU:HD13	1:A:105:PRO:CG	2.21	0.69
2:B:6:LYS:HG3	2:B:38:GLU:HG3	1.75	0.69
3:H:126:PRO:CD	3:H:188:TRP:HH2	2.05	0.69
3:H:142:VAL:CG2	3:H:177:LEU:HD11	2.22	0.69
5:U:134:GLU:HG2	5:U:135:GLU:N	2.07	0.69
1:A:22:ASN:HA	5:U:140:ASP:CG	2.18	0.69
3:H:77:THR:HG21	3:H:79:TYR:HE1	1.56	0.69
4:L:35:TRP:HZ3	4:L:88:CYS:SG	2.15	0.69
4:L:147:LYS:HB3	4:L:195:GLU:O	1.92	0.69
3:H:65:GLY:C	3:H:67:ALA:H	1.99	0.69
5:U:3:CYS:CA	5:U:75:LEU:HD23	2.22	0.69
2:B:3:GLU:HB3	2:B:19:CYS:SG	2.33	0.69
3:H:119:PRO:CD	3:H:199:HIS:HD2	2.04	0.69
4:L:6:GLN:OE1	4:L:101:GLY:N	2.19	0.69
4:L:8:PRO:HG2	4:L:11:LEU:HD22	1.75	0.69
4:L:35:TRP:CD1	4:L:48:ILE:CD1	2.62	0.69
3:H:4:LEU:CD2	3:H:22:CYS:SG	2.81	0.69
3:H:142:VAL:HG23	3:H:177:LEU:CD1	2.21	0.69
4:L:70:ASP:O	4:L:71:PHE:CD1	2.44	0.69
5:U:32:TRP:CZ2	5:U:34:GLU:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HD21	1:A:107:ASN:HA	1.55	0.69
4:L:211:ARG:HB3	4:L:211:ARG:CZ	2.23	0.69
5:U:126:VAL:HG22	5:U:143:HIS:NE2	2.08	0.69
3:H:143:LYS:HB2	3:H:176:THR:HG23	1.75	0.69
3:H:145:TYR:HE2	3:H:175:TYR:HB2	0.92	0.69
4:L:27(B):LEU:O	4:L:31:THR:HG23	1.92	0.69
4:L:116:SER:C	4:L:117:ILE:HD13	2.18	0.69
5:U:41:VAL:HG11	5:U:43:LYS:HE2	1.74	0.69
1:A:78:THR:HB	1:A:121:PRO:HG3	1.74	0.69
5:U:66:LEU:C	5:U:67:THR:HG22	2.17	0.69
5:U:239:ARG:HH12	5:U:274:PRO:HB3	1.58	0.69
5:U:137:ARG:CB	5:U:138:PRO:HD2	2.23	0.69
5:U:219:MET:HG2	5:U:242:ALA:HA	1.75	0.69
5:U:239:ARG:NH2	5:U:274:PRO:CA	2.54	0.69
1:A:41:HIS:C	1:A:42:CYS:SG	2.77	0.68
3:H:149:PRO:HG2	3:H:200:PRO:CD	2.23	0.68
5:U:125:VAL:O	5:U:125:VAL:HG13	1.93	0.68
3:H:47:TRP:CZ2	3:H:49:GLY:C	2.72	0.68
3:H:143:LYS:HG2	3:H:144:GLY:N	2.06	0.68
1:A:59:ARG:HB3	1:A:103:ARG:NH2	2.09	0.68
3:H:96:ILE:HG23	3:H:97:TYR:CA	2.19	0.68
3:H:150:VAL:HG22	3:H:198:ALA:O	1.94	0.68
4:L:145:ASN:O	4:L:196:ALA:HB1	1.93	0.68
5:U:26:THR:OG1	5:U:77:ASN:HB3	1.93	0.68
1:A:34:PRO:HB2	1:A:35:LYS:HE2	1.74	0.68
3:H:122:TYR:CE2	4:L:124:GLN:CG	2.76	0.68
5:U:213:ILE:O	5:U:213:ILE:HG12	1.91	0.68
1:A:63:SER:HB3	1:A:100:ASN:O	1.93	0.68
3:H:96:ILE:CG2	3:H:97:TYR:HA	2.17	0.68
3:H:146:PHE:HB2	3:H:174:LEU:HD23	1.74	0.68
4:L:83:LEU:HD23	4:L:84:GLY:N	2.09	0.68
3:H:188:TRP:CD1	3:H:189:PRO:CB	2.76	0.68
5:U:99:GLY:N	5:U:104:SER:HB3	2.01	0.68
1:A:35:LYS:O	1:A:37:PHE:N	2.26	0.68
3:H:170:LEU:CD1	3:H:171:GLN:N	2.51	0.68
1:A:71:CYS:HB2	1:A:100:ASN:O	1.94	0.68
3:H:21:SER:CB	3:H:23:LYS:NZ	2.56	0.68
1:A:57:PHE:HA	1:A:59:ARG:HH21	1.57	0.67
1:A:88:ARG:NH1	1:A:90:ASP:CG	2.51	0.67
2:B:22:ASP:OD1	2:B:22:ASP:C	2.36	0.67
3:H:3:GLN:O	3:H:24:ALA:HA	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:ND2	1:A:25:PHE:CE1	2.62	0.67
1:A:22:ASN:OD1	1:A:23:LYS:N	2.26	0.67
3:H:37:VAL:HG21	3:H:103:TRP:HZ3	1.58	0.67
4:L:35:TRP:CZ3	4:L:88:CYS:SG	2.87	0.67
4:L:147:LYS:HE3	4:L:154:GLU:CD	2.19	0.67
3:H:85:GLU:OE1	3:H:85:GLU:N	2.22	0.67
3:H:145:TYR:C	3:H:174:LEU:HD22	2.20	0.67
4:L:120:PRO:HG2	4:L:186:TYR:CE2	2.29	0.67
4:L:206:VAL:O	4:L:207:LYS:HD3	1.94	0.67
5:U:54:THR:HG22	5:U:55:LEU:N	2.08	0.67
5:U:203:HIS:HE2	6:D:1:NAG:C6	1.94	0.67
1:A:87:HIS:NE2	5:U:9:ASN:OD1	2.27	0.67
2:B:28:TYR:HD2	5:U:116:ARG:HG2	1.58	0.67
3:H:100(B):LEU:HD12	3:H:100(B):LEU:H	1.57	0.67
3:H:164:HIS:NE2	4:L:174:SER:OG	2.28	0.67
5:U:92:TYR:HB3	5:U:118:PRO:HA	1.76	0.67
5:U:157:ASN:HB2	5:U:245:SER:CB	2.25	0.67
5:U:159:PHE:CD2	5:U:160:HIS:N	2.63	0.67
3:H:149:PRO:HG2	3:H:200:PRO:HG2	1.77	0.67
4:L:142:LYS:H	4:L:142:LYS:CD	1.93	0.67
1:A:59:ARG:NH1	1:A:94:LEU:O	2.28	0.67
1:A:64:THR:N	1:A:71:CYS:SG	2.67	0.67
5:U:32:TRP:O	5:U:32:TRP:HE3	1.78	0.67
4:L:185:GLU:OE1	4:L:188:ARG:CD	2.43	0.67
5:U:29:VAL:HG13	5:U:66:LEU:HD22	1.76	0.67
5:U:92:TYR:N	5:U:92:TYR:CD1	2.63	0.67
5:U:198:LYS:O	5:U:204:GLY:O	2.14	0.66
3:H:2:VAL:HG21	3:H:102:TYR:CE2	2.30	0.66
3:H:33:TYR:CD2	3:H:52:ASN:ND2	2.63	0.66
5:U:37:GLU:HG3	5:U:37:GLU:O	1.87	0.66
3:H:116:THR:HA	3:H:147:PRO:HD3	1.77	0.66
3:H:145:TYR:CD2	3:H:145:TYR:C	2.72	0.66
1:A:81:GLN:OE1	1:A:81:GLN:HA	1.95	0.66
5:U:167:PHE:CE2	5:U:182:LEU:CD1	2.77	0.66
1:A:110:ARG:HB3	1:A:111:PRO:HD2	1.77	0.66
2:B:16:ASP:OD1	2:B:16:ASP:N	2.29	0.66
3:H:6:GLN:H	3:H:105:GLN:NE2	1.92	0.66
5:U:118:PRO:HG2	5:U:119:GLU:OE2	1.95	0.66
5:U:243:THR:OG1	5:U:245:SER:OG	2.14	0.66
1:A:51:TYR:HD2	1:A:51:TYR:N	1.91	0.66
3:H:188:TRP:CA	3:H:190:SER:H	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:73:LEU:HD12	4:L:74:LYS:N	2.11	0.66
4:L:117:ILE:O	4:L:118:PHE:HD1	1.77	0.66
5:U:25:ARG:HD3	5:U:68:GLU:OE1	1.96	0.66
3:H:188:TRP:HA	3:H:190:SER:N	2.11	0.66
4:L:90:GLN:O	4:L:90:GLN:CD	2.38	0.66
5:U:219:MET:CB	5:U:242:ALA:HA	2.25	0.66
4:L:35:TRP:HZ3	4:L:88:CYS:CB	1.94	0.66
5:U:152:GLY:C	5:U:154:PRO:HD2	2.20	0.66
5:U:167:PHE:HD2	5:U:182:LEU:HD12	1.58	0.66
4:L:76:SER:OG	4:L:77:ARG:N	2.26	0.66
3:H:144:GLY:C	3:H:174:LEU:HD13	2.20	0.66
4:L:105:GLU:C	4:L:106:LEU:HD22	2.20	0.66
3:H:192:THR:HG21	3:H:209:LYS:HZ1	1.59	0.65
1:A:24:TYR:O	5:U:53:ARG:HD2	1.96	0.65
3:H:36:TRP:HZ2	3:H:79:TYR:O	1.79	0.65
3:H:116:THR:HG21	3:H:201:ALA:O	1.95	0.65
3:H:152:VAL:CB	3:H:197:VAL:HG23	2.26	0.65
3:H:180:SER:HB3	4:L:135:PHE:HE1	1.58	0.65
4:L:116:SER:CB	4:L:118:PHE:CE1	2.70	0.65
4:L:188:ARG:C	4:L:189:HIS:ND1	2.54	0.65
3:H:52:ASN:OD1	3:H:52:ASN:O	2.14	0.65
5:U:159:PHE:CD2	5:U:159:PHE:C	2.73	0.65
1:A:117:VAL:HG12	1:A:122:LEU:HD22	1.77	0.65
3:H:31:SER:C	5:U:212:LEU:HD13	2.22	0.65
3:H:33:TYR:C	3:H:96:ILE:HD11	2.21	0.65
2:B:27:TYR:HE2	5:U:116:ARG:HD2	1.59	0.65
2:B:28:TYR:OH	5:U:114:GLN:HB2	1.96	0.65
3:H:48:ILE:HG22	3:H:49:GLY:N	2.09	0.65
3:H:60:ASN:OD1	3:H:62:LYS:HG2	1.97	0.65
5:U:62:LYS:NZ	5:U:62:LYS:HB3	2.11	0.65
5:U:96:ILE:CG2	5:U:110:HIS:HB3	2.26	0.65
1:A:51:TYR:N	1:A:51:TYR:CD2	2.63	0.65
2:B:27:TYR:CD1	5:U:63:ILE:CD1	2.72	0.65
3:H:166:PHE:CZ	4:L:175:MET:O	2.50	0.65
4:L:70:ASP:C	4:L:71:PHE:CD1	2.74	0.65
3:H:68:THR:HB	3:H:81:GLN:HB3	1.79	0.65
3:H:143:LYS:CG	3:H:176:THR:OG1	2.43	0.65
5:U:173:THR:HG23	5:U:176:CYS:HB3	1.79	0.65
2:B:27:TYR:C	2:B:27:TYR:HD2	2.04	0.65
4:L:186:TYR:CE1	4:L:192:TYR:CE2	2.82	0.65
5:U:9:ASN:OD1	5:U:10:GLY:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:303:MAN:C2	6:C:2:NAG:H62	2.27	0.65
1:A:92:LEU:CD2	1:A:92:LEU:N	2.59	0.65
5:U:123:LEU:CD1	5:U:146:GLY:O	2.45	0.65
1:A:86:ALA:HB2	1:A:96:LEU:HB3	1.79	0.65
5:U:97:SER:CA	5:U:145:ARG:O	2.44	0.65
1:A:34:PRO:O	1:A:36:LYS:N	2.30	0.64
1:A:72:LEU:CD2	1:A:116:GLN:H	2.00	0.64
5:U:190:ASN:CG	5:U:215:CYS:HB2	2.22	0.64
1:A:79:VAL:HG13	1:A:114:TYR:CD2	2.32	0.64
4:L:7:THR:CG2	4:L:8:PRO:CA	2.75	0.64
4:L:37:LEU:CD1	4:L:38:GLN:N	2.57	0.64
5:U:92:TYR:CB	5:U:118:PRO:HA	2.26	0.64
5:U:96:ILE:HG21	5:U:110:HIS:HB3	1.78	0.64
2:B:28:TYR:HB2	2:B:30:SER:OG	1.96	0.64
3:H:6:GLN:N	3:H:105:GLN:HE22	1.96	0.64
3:H:50:GLU:C	3:H:51:ILE:HG22	2.21	0.64
4:L:46:ARG:NH1	4:L:49:TYR:CE1	2.66	0.64
5:U:92:TYR:CD2	5:U:118:PRO:HB3	2.33	0.64
3:H:152:VAL:CG2	3:H:197:VAL:CG2	2.56	0.64
1:A:14:LEU:HB3	1:A:15:ASN:OD1	1.97	0.64
1:A:95:GLY:C	1:A:96:LEU:HD23	2.23	0.64
3:H:29:PHE:HD2	3:H:76:ARG:HA	1.61	0.64
1:A:110:ARG:HH21	1:A:125:GLU:HG2	1.62	0.64
2:B:40:LYS:HZ2	5:U:35:GLY:HA3	1.63	0.64
3:H:2:VAL:HG11	3:H:102:TYR:CG	2.33	0.64
3:H:63:ILE:CG2	3:H:65:GLY:H	2.02	0.64
1:A:34:PRO:O	1:A:35:LYS:C	2.41	0.64
1:A:99:HIS:CD2	1:A:101:TYR:HB2	2.32	0.64
2:B:19:CYS:C	2:B:32:CYS:SG	2.81	0.64
4:L:191:SER:CB	4:L:210:ASN:ND2	2.57	0.64
5:U:61:LEU:CD1	5:U:61:LEU:H	2.00	0.64
3:H:6:GLN:CB	3:H:105:GLN:NE2	2.53	0.64
4:L:27(A):SER:OG	4:L:27(B):LEU:N	2.29	0.64
4:L:34:ASN:OD1	4:L:34:ASN:N	2.31	0.64
4:L:115:VAL:HG22	4:L:136:LEU:HD23	1.80	0.64
4:L:194:CYS:O	4:L:206:VAL:HG13	1.97	0.64
1:A:35:LYS:CG	1:A:36:LYS:H	2.09	0.64
3:H:94:ARG:CB	3:H:96:ILE:HD12	2.27	0.64
3:H:178:SER:CB	4:L:176:SER:HG	2.11	0.64
5:U:230:GLU:HB3	5:U:231:PRO:HD3	1.79	0.64
3:H:6:GLN:CG	3:H:105:GLN:HE22	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:24:LYS:HD2	4:L:24:LYS:N	2.13	0.64
5:U:223:LEU:HD23	5:U:224:VAL:N	2.13	0.64
1:A:15:ASN:CG	1:A:37:PHE:HE1	2.04	0.63
3:H:193:VAL:HG12	3:H:210:ILE:HG12	1.79	0.63
5:U:157:ASN:CB	5:U:245:SER:OG	2.46	0.63
1:A:85:HIS:NE2	1:A:87:HIS:O	2.31	0.63
3:H:122:TYR:CG	4:L:124:GLN:HB2	2.33	0.63
4:L:13:VAL:HG12	4:L:14:THR:N	2.11	0.63
4:L:59:PRO:HG2	4:L:62:PHE:CE1	2.32	0.63
5:U:246:MET:HE3	5:U:252:LEU:HD12	1.80	0.63
1:A:72:LEU:N	1:A:72:LEU:CD2	2.59	0.63
2:B:19:CYS:C	2:B:20:GLN:OE1	2.41	0.63
3:H:12:VAL:HB	3:H:111:VAL:HG12	1.79	0.63
5:U:203:HIS:NE2	6:D:1:NAG:H61	2.12	0.63
3:H:4:LEU:HD22	3:H:22:CYS:SG	2.38	0.63
4:L:4:MET:HG2	4:L:97:THR:HB	1.81	0.63
4:L:89:TRP:HB3	4:L:98:PHE:HD2	1.61	0.63
5:U:4:MET:CE	5:U:78:GLN:HB2	2.29	0.63
5:U:252:LEU:HG	5:U:256:PHE:CD1	2.34	0.63
1:A:43:GLU:C	1:A:44:ILE:HD12	2.22	0.63
1:A:92:LEU:HD23	1:A:92:LEU:N	2.08	0.63
1:A:22:ASN:HD21	1:A:25:PHE:HE1	1.46	0.63
3:H:80:MET:HE2	3:H:82:PHE:HD1	1.63	0.63
5:U:189:GLN:HA	5:U:189:GLN:OE1	1.98	0.63
2:B:13:PHE:HE1	2:B:20:GLN:NE2	1.96	0.63
3:H:4:LEU:HD21	3:H:22:CYS:SG	2.39	0.63
5:U:94:GLU:HG3	5:U:95:CYS:N	2.12	0.63
5:U:190:ASN:ND2	5:U:215:CYS:C	2.57	0.63
5:U:203:HIS:NE2	6:D:1:NAG:O6	2.26	0.63
5:U:199:GLY:C	5:U:204:GLY:HA3	2.24	0.63
5:U:227:GLY:HA3	5:U:261:ILE:HG22	1.80	0.63
2:B:27:TYR:CE1	5:U:63:ILE:HG21	2.34	0.63
3:H:2:VAL:HG11	3:H:102:TYR:HB3	1.81	0.63
3:H:41:HIS:C	3:H:43:LYS:N	2.57	0.63
1:A:61:LYS:HA	1:A:101:TYR:CB	2.29	0.62
3:H:45:LEU:C	3:H:46:GLU:HG3	2.23	0.62
5:U:52:ASN:OD1	5:U:69:VAL:HG23	1.99	0.62
5:U:167:PHE:CE2	5:U:182:LEU:HD12	2.34	0.62
1:A:14:LEU:CB	1:A:15:ASN:OD1	2.48	0.62
3:H:80:MET:CE	3:H:82:PHE:HD1	2.12	0.62
5:U:197:CYS:SG	5:U:239:ARG:HG3	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:41:HIS:C	3:H:43:LYS:H	2.04	0.62
5:U:184:LEU:O	5:U:185:GLU:C	2.42	0.62
1:A:44:ILE:HG21	1:A:60:GLY:H	1.60	0.62
1:A:63:SER:O	1:A:64:THR:HG22	1.98	0.62
3:H:43:LYS:HA	3:H:43:LYS:CE	2.29	0.62
3:H:149:PRO:HG2	3:H:200:PRO:CG	2.30	0.62
4:L:12:SER:OG	4:L:105:GLU:HB2	1.99	0.62
5:U:30:ARG:HD3	5:U:116:ARG:HH12	1.65	0.62
5:U:157:ASN:CB	5:U:245:SER:CB	2.76	0.62
1:A:14:LEU:O	1:A:17:GLY:N	2.32	0.62
3:H:149:PRO:CG	3:H:200:PRO:HG2	2.30	0.62
5:U:132:GLU:HG3	5:U:136:GLY:H	1.64	0.62
1:A:55:GLY:C	1:A:57:PHE:H	2.08	0.62
3:H:2:VAL:CG1	3:H:102:TYR:CD2	2.83	0.62
3:H:63:ILE:O	3:H:64:LYS:HB2	1.99	0.62
3:H:100(A):VAL:HA	4:L:89:TRP:HH2	1.64	0.62
5:U:191:GLY:O	5:U:193:GLN:NE2	2.33	0.62
5:U:205:CYS:CB	5:U:237:MET:SD	2.88	0.62
4:L:185:GLU:O	4:L:188:ARG:HG3	1.98	0.62
4:L:65:SER:OG	4:L:72:THR:HB	1.99	0.62
3:H:197:VAL:HG12	3:H:206:VAL:CG1	2.29	0.62
5:U:57:TYR:CD1	5:U:144:LEU:HD11	2.35	0.62
1:A:36:LYS:C	1:A:37:PHE:HD2	2.08	0.61
2:B:24:LEU:HD13	2:B:28:TYR:OH	1.99	0.61
2:B:28:TYR:CE1	5:U:91:ARG:CZ	2.83	0.61
4:L:48:ILE:HG23	4:L:54:LEU:HD23	1.82	0.61
4:L:179:LEU:HB3	4:L:181:LEU:HD11	1.82	0.61
5:U:7:LYS:HE3	5:U:11:ASP:CB	2.30	0.61
1:A:84:TYR:HD2	1:A:88:ARG:HH21	1.48	0.61
1:A:117:VAL:CG1	1:A:122:LEU:HD22	2.30	0.61
3:H:29:PHE:HE1	3:H:34:MET:HE3	1.65	0.61
3:H:154:TRP:CD1	3:H:181:VAL:HG11	2.35	0.61
5:U:137:ARG:HH22	5:U:198:LYS:HZ2	1.46	0.61
5:U:167:PHE:HE2	5:U:182:LEU:HD11	1.65	0.61
1:A:88:ARG:O	1:A:90:ASP:N	2.33	0.61
4:L:61:ARG:HD2	4:L:77:ARG:HB2	1.81	0.61
4:L:140:TYR:CG	4:L:141:PRO:HA	2.35	0.61
5:U:41:VAL:CG1	5:U:43:LYS:HE2	2.29	0.61
1:A:65:ASP:OD1	1:A:69:ARG:N	2.32	0.61
3:H:126:PRO:HD2	3:H:188:TRP:CH2	2.29	0.61
5:U:32:TRP:C	5:U:32:TRP:HE3	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:123:LEU:HA	5:U:169:LYS:O	2.00	0.61
3:H:50:GLU:OE2	4:L:94:PHE:CE1	2.53	0.61
3:H:145:TYR:O	3:H:145:TYR:HD2	1.83	0.61
4:L:9:LEU:H	4:L:9:LEU:CD1	2.11	0.61
4:L:70:ASP:OD1	4:L:71:PHE:N	2.33	0.61
1:A:52:GLU:O	1:A:55:GLY:N	2.29	0.61
3:H:169:VAL:HG11	4:L:160:LEU:HD13	1.82	0.61
4:L:6:GLN:CG	4:L:100:ALA:H	2.13	0.61
4:L:135:PHE:O	4:L:136:LEU:HD23	1.99	0.61
2:B:32:CYS:O	2:B:33:THR:C	2.42	0.61
3:H:2:VAL:HG11	3:H:102:TYR:HD2	1.65	0.61
3:H:180:SER:CB	4:L:135:PHE:CE1	2.83	0.61
5:U:195:TYR:H	5:U:272:ASN:ND2	1.98	0.61
4:L:151:ASP:OD2	4:L:189:HIS:CB	2.49	0.61
5:U:69:VAL:HG22	5:U:70:VAL:N	2.15	0.61
2:B:28:TYR:HE1	5:U:91:ARG:CZ	2.14	0.61
3:H:6:GLN:HG3	3:H:105:GLN:NE2	2.15	0.61
3:H:78:ALA:O	3:H:79:TYR:HD1	1.83	0.61
3:H:142:VAL:HB	3:H:177:LEU:HG	1.81	0.61
4:L:33:LEU:HD23	4:L:90:GLN:HB3	1.81	0.61
3:H:188:TRP:CZ2	3:H:212:PRO:CG	2.81	0.60
1:A:31:CYS:HB3	1:A:42:CYS:SG	2.41	0.60
1:A:86:ALA:HB2	1:A:96:LEU:CB	2.30	0.60
3:H:154:TRP:CD1	3:H:163:VAL:CG1	2.82	0.60
5:U:195:TYR:HB2	5:U:272:ASN:ND2	2.16	0.60
2:B:31:CYS:SG	2:B:35:TYR:CD2	2.94	0.60
3:H:29:PHE:C	3:H:31:SER:N	2.57	0.60
4:L:17:GLN:O	4:L:78:VAL:CG2	2.47	0.60
1:A:75:ASN:HB2	1:A:98:LYS:HA	1.81	0.60
3:H:33:TYR:N	3:H:96:ILE:CD1	2.65	0.60
3:H:144:GLY:C	3:H:174:LEU:HD22	2.27	0.60
4:L:133:VAL:CG1	4:L:135:PHE:CD2	2.84	0.60
5:U:120:GLU:HA	5:U:148:GLY:O	2.02	0.60
3:H:47:TRP:CZ2	3:H:49:GLY:HA2	2.33	0.60
5:U:233:ASN:O	5:U:233:ASN:ND2	2.28	0.60
2:B:28:TYR:HD2	5:U:116:ARG:CG	2.14	0.60
3:H:122:TYR:HB2	3:H:141:LEU:HB3	1.83	0.60
4:L:34:ASN:OD1	4:L:89:TRP:O	2.19	0.60
4:L:90:GLN:HG3	4:L:97:THR:OG1	2.01	0.60
5:U:126:VAL:CG2	5:U:143:HIS:NE2	2.65	0.60
3:H:59:TYR:OH	3:H:68:THR:CA	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:TRP:O	3:H:157:GLY:N	2.34	0.60
1:A:25:PHE:HD1	1:A:25:PHE:H	1.48	0.60
1:A:130:ASP:CG	1:A:131:CYS:N	2.57	0.60
2:B:13:PHE:CE1	2:B:20:GLN:CG	2.85	0.60
4:L:33:LEU:HB3	4:L:51:VAL:HG23	1.81	0.60
4:L:108:ARG:HD3	4:L:172:THR:HG22	1.83	0.60
5:U:167:PHE:HE2	5:U:182:LEU:CD1	2.15	0.60
5:U:205:CYS:SG	5:U:237:MET:SD	3.00	0.60
3:H:34:MET:O	3:H:50:GLU:HA	2.01	0.59
4:L:47:LEU:HD21	4:L:62:PHE:CD2	2.36	0.59
4:L:2:VAL:HG22	4:L:97:THR:HG21	1.83	0.59
1:A:99:HIS:CD2	1:A:99:HIS:C	2.78	0.59
3:H:188:TRP:NE1	3:H:212:PRO:HG2	2.17	0.59
1:A:47:SER:OG	1:A:48:LYS:N	2.35	0.59
3:H:38:LYS:HG3	3:H:90:TYR:HE1	1.67	0.59
4:L:115:VAL:CG1	4:L:117:ILE:HD11	2.33	0.59
5:U:30:ARG:NH2	5:U:37:GLU:OE2	2.35	0.59
3:H:4:LEU:HA	3:H:23:LYS:O	2.02	0.59
3:H:65:GLY:C	3:H:67:ALA:N	2.59	0.59
3:H:123:PRO:HD3	3:H:208:LYS:HE2	1.83	0.59
4:L:37:LEU:HD11	4:L:38:GLN:C	2.28	0.59
5:U:237:MET:HE1	5:U:239:ARG:NH1	2.17	0.59
4:L:105:GLU:O	4:L:106:LEU:HD13	2.01	0.59
4:L:195:GLU:HB3	4:L:206:VAL:CG2	2.24	0.59
4:L:140:TYR:CB	4:L:172:THR:HG22	2.30	0.59
1:A:40:GLN:OE1	5:U:8:THR:HG22	2.03	0.59
1:A:51:TYR:CD1	1:A:111:PRO:CD	2.86	0.59
1:A:119:LEU:HD13	1:A:119:LEU:O	2.03	0.59
3:H:33:TYR:CD1	3:H:50:GLU:OE1	2.55	0.59
4:L:82:ASP:N	4:L:82:ASP:OD1	2.36	0.59
5:U:25:ARG:CG	5:U:46:THR:HB	2.29	0.59
1:A:76:SER:OG	1:A:79:VAL:CG2	2.45	0.59
1:A:99:HIS:CD2	1:A:101:TYR:CB	2.86	0.59
4:L:37:LEU:HB2	4:L:86:TYR:CE1	2.38	0.59
5:U:160:HIS:NE2	5:U:215:CYS:HA	2.18	0.59
5:U:161:ASN:HB2	5:U:196:SER:HB2	1.85	0.59
1:A:55:GLY:C	1:A:57:PHE:N	2.57	0.58
3:H:21:SER:CB	3:H:23:LYS:HZ1	2.12	0.58
4:L:136:LEU:HD13	4:L:144:ILE:HD13	1.84	0.58
4:L:186:TYR:HE1	4:L:192:TYR:CE2	2.13	0.58
5:U:18:ALA:O	5:U:19:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:52:ASN:CG	5:U:69:VAL:HG23	2.29	0.58
1:A:23:LYS:HB2	5:U:255:ALA:HA	1.85	0.58
1:A:54:ASN:OD1	1:A:56:HIS:HB2	2.02	0.58
1:A:84:TYR:CD2	1:A:88:ARG:NH2	2.68	0.58
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.68	0.58
3:H:33:TYR:CZ	3:H:98:GLY:CA	2.84	0.58
3:H:38:LYS:HD3	3:H:40:SER:HB3	1.85	0.58
3:H:154:TRP:CD1	3:H:181:VAL:CG1	2.86	0.58
5:U:55:LEU:HD23	5:U:55:LEU:C	2.28	0.58
5:U:184:LEU:CD1	5:U:216:ARG:HD3	2.33	0.58
1:A:15:ASN:OD1	1:A:15:ASN:N	2.36	0.58
1:A:83:THR:HG22	1:A:84:TYR:N	2.18	0.58
3:H:59:TYR:CE1	3:H:69:PHE:CD2	2.91	0.58
4:L:37:LEU:HD21	4:L:39:ARG:CG	2.23	0.58
4:L:37:LEU:CD1	4:L:38:GLN:C	2.77	0.58
2:B:19:CYS:O	2:B:32:CYS:SG	2.61	0.58
4:L:40:PRO:HD3	4:L:84:GLY:HA2	1.86	0.58
4:L:138:ASN:HD22	4:L:170:ASP:CG	2.11	0.58
4:L:190:ASN:CG	4:L:211:ARG:HB2	2.27	0.58
1:A:110:ARG:HB3	1:A:111:PRO:CD	2.33	0.58
3:H:188:TRP:CD1	3:H:189:PRO:HB3	2.39	0.58
5:U:205:CYS:HB3	5:U:237:MET:SD	2.43	0.58
3:H:5:GLN:O	3:H:23:LYS:N	2.36	0.58
4:L:32:TYR:O	4:L:33:LEU:C	2.47	0.58
4:L:149:LYS:HD2	4:L:195:GLU:OE2	2.04	0.58
5:U:93:LEU:HD23	5:U:120:GLU:O	2.03	0.58
5:U:173:THR:HG23	5:U:176:CYS:CB	2.33	0.58
5:U:273:HIS:CD2	5:U:274:PRO:HD2	2.37	0.58
2:B:13:PHE:CE1	2:B:20:GLN:NE2	2.72	0.58
3:H:31:SER:C	3:H:32:TYR:CD1	2.82	0.58
3:H:146:PHE:HB3	3:H:174:LEU:CD2	2.31	0.58
5:U:27:THR:OG1	5:U:68:GLU:HG3	2.03	0.58
1:A:24:TYR:O	5:U:53:ARG:CD	2.52	0.58
1:A:25:PHE:O	1:A:27:ASN:N	2.36	0.57
3:H:4:LEU:HB3	3:H:104:GLY:HA3	1.86	0.57
3:H:101:ASP:CG	3:H:102:TYR:H	2.12	0.57
3:H:208:LYS:NZ	4:L:123:GLU:OE1	2.29	0.57
4:L:28:ASP:CG	4:L:28:ASP:O	2.47	0.57
5:U:99:GLY:O	5:U:104:SER:HB3	2.04	0.57
1:A:24:TYR:C	1:A:25:PHE:CD1	2.81	0.57
4:L:37:LEU:HD11	4:L:38:GLN:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:139:PHE:CE2	4:L:144:ILE:HB	2.35	0.57
5:U:238:VAL:HG12	5:U:239:ARG:N	2.18	0.57
1:A:51:TYR:OH	1:A:130:ASP:HB2	2.04	0.57
4:L:132:VAL:O	4:L:132:VAL:HG12	2.00	0.57
3:H:6:GLN:HG3	3:H:105:GLN:HE22	1.69	0.57
3:H:164:HIS:CD2	4:L:174:SER:OG	2.58	0.57
3:H:170:LEU:HB2	3:H:175:TYR:CD2	2.39	0.57
5:U:25:ARG:HG2	5:U:46:THR:CB	2.30	0.57
5:U:97:SER:HB2	5:U:146:GLY:HA2	1.86	0.57
5:U:200:ASN:O	5:U:201:SER:C	2.46	0.57
1:A:23:LYS:HG2	5:U:140:ASP:OD1	2.04	0.57
3:H:33:TYR:CA	3:H:96:ILE:HG12	2.34	0.57
3:H:36:TRP:HA	3:H:91:TYR:O	2.05	0.57
3:H:51:ILE:HG21	3:H:69:PHE:CB	2.35	0.57
3:H:78:ALA:O	3:H:79:TYR:CD1	2.57	0.57
4:L:148:TRP:CD1	4:L:179:LEU:CD2	2.88	0.57
5:U:133:GLY:HA3	5:U:137:ARG:HE	1.62	0.57
5:U:163:ASP:C	5:U:163:ASP:OD1	2.48	0.57
1:A:51:TYR:CD1	1:A:111:PRO:HD3	2.40	0.57
1:A:65:ASP:OD1	1:A:68:GLY:N	2.37	0.57
1:A:80:LEU:HD23	1:A:85:HIS:NE2	2.20	0.57
2:B:6:LYS:HA	2:B:38:GLU:HG3	1.86	0.57
3:H:33:TYR:CE2	3:H:98:GLY:CA	2.88	0.57
4:L:92:THR:O	4:L:92:THR:HG22	2.05	0.57
5:U:172:ASN:HD22	8:U:304:NAG:C7	1.98	0.57
1:A:20:VAL:HA	5:U:139:LYS:HB3	1.86	0.57
1:A:61:LYS:HA	1:A:101:TYR:HB3	1.85	0.57
3:H:47:TRP:CZ2	3:H:49:GLY:CA	2.87	0.57
5:U:252:LEU:HG	5:U:256:PHE:HE1	1.70	0.57
1:A:51:TYR:CE2	1:A:129:HIS:O	2.57	0.57
1:A:69:ARG:HB3	1:A:70:PRO:CD	2.34	0.57
1:A:119:LEU:HD13	1:A:119:LEU:C	2.29	0.57
2:B:5:CYS:N	2:B:34:ASP:OD1	2.38	0.57
2:B:28:TYR:C	2:B:29:GLN:HG3	2.29	0.57
3:H:33:TYR:HB2	3:H:95:SER:HB3	1.86	0.57
4:L:190:ASN:HA	4:L:211:ARG:HG3	1.87	0.57
5:U:102:ASP:OD1	5:U:104:SER:HB2	2.05	0.57
1:A:61:LYS:O	1:A:62:ALA:HB3	2.05	0.57
1:A:99:HIS:CD2	1:A:101:TYR:CA	2.88	0.57
2:B:6:LYS:CG	2:B:38:GLU:HG3	2.35	0.57
3:H:101:ASP:N	3:H:101:ASP:OD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:LYS:HE3	3:H:113:SER:HA	1.86	0.56
3:H:80:MET:CE	3:H:82:PHE:CD1	2.88	0.56
5:U:168:LEU:HD13	5:U:168:LEU:C	2.29	0.56
1:A:46:LYS:HB3	1:A:61:LYS:HE2	1.87	0.56
1:A:88:ARG:O	1:A:91:ALA:N	2.37	0.56
1:A:90:ASP:O	1:A:91:ALA:C	2.48	0.56
3:H:2:VAL:CB	3:H:102:TYR:CD2	2.88	0.56
3:H:83:THR:O	3:H:86:ASP:CB	2.50	0.56
3:H:184:PRO:HD2	3:H:187:THR:OG1	2.05	0.56
4:L:37:LEU:CD2	4:L:39:ARG:HG3	2.25	0.56
4:L:105:GLU:HB3	4:L:166:GLN:HE22	1.70	0.56
5:U:28:ILE:HG13	5:U:40:LEU:O	2.05	0.56
5:U:93:LEU:O	5:U:115:CYS:SG	2.63	0.56
5:U:152:GLY:C	5:U:154:PRO:CD	2.78	0.56
5:U:223:LEU:HD23	5:U:223:LEU:C	2.30	0.56
3:H:99:HIS:O	3:H:100:SER:C	2.47	0.56
3:H:105:GLN:HA	4:L:43:SER:HB3	1.87	0.56
4:L:135:PHE:HB3	4:L:137:ASN:OD1	2.06	0.56
5:U:230:GLU:O	5:U:232:LYS:N	2.39	0.56
3:H:111:VAL:HG23	3:H:111:VAL:O	2.04	0.56
4:L:106:LEU:N	4:L:106:LEU:CD2	2.67	0.56
4:L:138:ASN:CA	4:L:173:TYR:O	2.53	0.56
5:U:133:GLY:CA	5:U:137:ARG:NE	2.64	0.56
5:U:160:HIS:CE1	5:U:215:CYS:HA	2.40	0.56
5:U:205:CYS:SG	5:U:237:MET:HE2	2.45	0.56
1:A:95:GLY:HA3	1:A:103:ARG:HE	1.70	0.56
3:H:154:TRP:NE1	3:H:181:VAL:HG12	2.20	0.56
5:U:225:ALA:O	5:U:237:MET:HA	2.05	0.56
1:A:59:ARG:NH1	1:A:94:LEU:C	2.63	0.56
3:H:53:TYR:HE2	5:U:214:ASP:CG	2.13	0.56
5:U:219:MET:CG	5:U:242:ALA:HA	2.34	0.56
5:U:274:PRO:O	5:U:275:ASP:HB2	2.06	0.56
1:A:71:CYS:O	1:A:72:LEU:C	2.49	0.56
5:U:17:CYS:O	5:U:18:ALA:C	2.49	0.56
1:A:72:LEU:HD11	1:A:116:GLN:HB2	1.86	0.56
3:H:95:SER:CB	3:H:96:ILE:CA	2.84	0.56
3:H:177:LEU:C	3:H:177:LEU:HD12	2.31	0.56
4:L:94:PHE:N	4:L:94:PHE:CD2	2.73	0.56
4:L:139:PHE:HE2	4:L:144:ILE:CB	2.18	0.56
4:L:170:ASP:C	4:L:172:THR:H	2.13	0.56
5:U:61:LEU:HD12	5:U:61:LEU:H	1.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:184:LEU:C	5:U:186:ASN:H	2.13	0.56
5:U:246:MET:CE	5:U:252:LEU:HD12	2.36	0.56
2:B:7:GLY:C	2:B:9:CYS:N	2.52	0.56
3:H:166:PHE:CE2	4:L:175:MET:N	2.74	0.56
5:U:167:PHE:CD1	5:U:168:LEU:N	2.74	0.56
1:A:34:PRO:C	1:A:35:LYS:CG	2.79	0.55
1:A:97:GLY:O	1:A:99:HIS:N	2.39	0.55
3:H:29:PHE:HE1	3:H:34:MET:CE	2.19	0.55
3:H:165:THR:HG22	3:H:166:PHE:N	2.21	0.55
5:U:219:MET:HB3	5:U:242:ALA:C	2.29	0.55
3:H:145:TYR:HE1	3:H:150:VAL:CG2	2.20	0.55
4:L:49:TYR:O	4:L:50:LEU:CB	2.53	0.55
5:U:51:THR:H	5:U:53:ARG:HH21	1.54	0.55
1:A:43:GLU:O	1:A:44:ILE:HG13	2.07	0.55
1:A:59:ARG:CA	1:A:103:ARG:NH1	2.69	0.55
4:L:51:VAL:CG2	4:L:71:PHE:HE2	2.18	0.55
4:L:142:LYS:HD2	4:L:173:TYR:CE1	2.42	0.55
5:U:62:LYS:HB3	5:U:62:LYS:HZ2	1.72	0.55
5:U:194:CYS:SG	5:U:215:CYS:SG	3.04	0.55
2:B:27:TYR:HE2	5:U:116:ARG:HG3	1.71	0.55
5:U:187:LEU:HB3	5:U:188:PRO:CD	2.33	0.55
3:H:148:GLU:OE1	3:H:149:PRO:HA	2.05	0.55
4:L:33:LEU:HD22	4:L:34:ASN:N	2.22	0.55
4:L:61:ARG:O	4:L:75:ILE:HA	2.06	0.55
4:L:190:ASN:OD1	4:L:211:ARG:CB	2.42	0.55
7:U:303:MAN:H2	6:C:2:NAG:H62	1.88	0.55
1:A:94:LEU:HD23	1:A:94:LEU:N	2.03	0.55
3:H:36:TRP:O	3:H:48:ILE:HB	2.06	0.55
3:H:188:TRP:NE1	3:H:189:PRO:HB3	2.22	0.55
4:L:150:ILE:HD12	4:L:155:ARG:HH11	1.69	0.55
5:U:159:PHE:CG	5:U:160:HIS:N	2.74	0.55
5:U:196:SER:HB2	5:U:213:ILE:HD12	1.89	0.55
1:A:123:VAL:O	1:A:123:VAL:HG13	2.05	0.55
3:H:32:TYR:CE2	3:H:94:ARG:NH2	2.74	0.55
3:H:116:THR:HA	3:H:147:PRO:CD	2.36	0.55
4:L:48:ILE:HG23	4:L:54:LEU:CD2	2.35	0.55
5:U:202:THR:O	5:U:203:HIS:ND1	2.40	0.55
1:A:72:LEU:CD2	1:A:114:TYR:O	2.54	0.55
3:H:6:GLN:CA	3:H:105:GLN:HE22	2.19	0.55
3:H:193:VAL:HG12	3:H:210:ILE:CG1	2.36	0.55
4:L:166:GLN:HG3	4:L:171:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:180:THR:CA	4:L:181:LEU:HG	2.37	0.55
4:L:206:VAL:O	4:L:207:LYS:CD	2.55	0.55
5:U:43:LYS:HD3	5:U:77:ASN:O	2.06	0.55
5:U:109:ARG:O	5:U:110:HIS:C	2.50	0.55
1:A:46:LYS:HB3	1:A:61:LYS:CE	2.37	0.54
1:A:56:HIS:CB	1:A:57:PHE:CD1	2.64	0.54
1:A:106:ASP:OD2	1:A:108:ARG:HG3	2.07	0.54
1:A:34:PRO:C	1:A:35:LYS:HG2	2.31	0.54
3:H:2:VAL:CG2	3:H:102:TYR:CD2	2.90	0.54
3:H:33:TYR:HD1	3:H:50:GLU:OE1	1.90	0.54
3:H:152:VAL:HG22	3:H:197:VAL:HG22	1.81	0.54
4:L:33:LEU:HD22	4:L:34:ASN:H	1.73	0.54
1:A:85:HIS:CD2	1:A:86:ALA:N	2.74	0.54
1:A:115:VAL:O	1:A:116:GLN:C	2.50	0.54
3:H:31:SER:O	5:U:212:LEU:CD1	2.56	0.54
3:H:32:TYR:CA	3:H:96:ILE:HD13	2.35	0.54
3:H:97:TYR:CE2	5:U:212:LEU:HD22	2.39	0.54
4:L:190:ASN:OD1	4:L:211:ARG:N	2.35	0.54
5:U:71:CYS:SG	5:U:73:LEU:HD21	2.47	0.54
3:H:72:ASP:CB	3:H:75:SER:OG	2.55	0.54
3:H:97:TYR:HB3	5:U:270:GLY:HA3	1.90	0.54
5:U:225:ALA:HB2	5:U:263:VAL:HG12	1.90	0.54
5:U:226:THR:O	5:U:261:ILE:HA	2.07	0.54
1:A:56:HIS:CB	1:A:57:PHE:CE1	2.89	0.54
3:H:14:THR:HG23	3:H:83:THR:HA	1.89	0.54
3:H:144:GLY:HA2	3:H:174:LEU:CD1	2.17	0.54
3:H:145:TYR:HE2	3:H:175:TYR:HB3	1.65	0.54
4:L:13:VAL:HG12	4:L:14:THR:O	2.07	0.54
5:U:167:PHE:CD2	5:U:182:LEU:CD1	2.89	0.54
1:A:59:ARG:CA	1:A:103:ARG:CZ	2.83	0.54
2:B:27:TYR:CD2	5:U:116:ARG:HD2	2.42	0.54
3:H:29:PHE:CE1	3:H:34:MET:HE3	2.42	0.54
3:H:167:PRO:O	3:H:168:ALA:C	2.49	0.54
4:L:108:ARG:CD	4:L:172:THR:HG23	2.32	0.54
5:U:30:ARG:HD3	5:U:116:ARG:NH1	2.22	0.54
5:U:109:ARG:O	5:U:111:GLN:HG3	2.07	0.54
5:U:128:HIS:HB2	5:U:165:PHE:HB3	1.89	0.54
1:A:73:PRO:HA	1:A:100:ASN:CA	2.34	0.54
1:A:114:TYR:HA	1:A:122:LEU:O	2.06	0.54
3:H:51:ILE:HG21	3:H:69:PHE:HB3	1.89	0.54
4:L:190:ASN:O	4:L:210:ASN:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:165:PHE:CE1	5:U:184:LEU:HB2	2.43	0.54
1:A:77:ALA:O	1:A:79:VAL:N	2.41	0.54
3:H:12:VAL:CB	3:H:111:VAL:HG12	2.37	0.54
3:H:192:THR:CB	3:H:209:LYS:CE	2.69	0.54
4:L:28:ASP:OD2	4:L:30:LYS:HG3	2.07	0.54
5:U:133:GLY:CA	5:U:137:ARG:NH2	2.71	0.54
5:U:203:HIS:CE1	6:D:1:NAG:C5	2.90	0.54
2:B:40:LYS:N	2:B:41:PRO:HD3	2.20	0.54
3:H:80:MET:HE2	3:H:82:PHE:CD1	2.43	0.54
1:A:91:ALA:O	1:A:92:LEU:C	2.51	0.54
1:A:91:ALA:O	1:A:93:GLN:N	2.41	0.54
1:A:97:GLY:C	1:A:99:HIS:N	2.63	0.54
3:H:11:LEU:HG	3:H:12:VAL:N	2.02	0.54
3:H:95:SER:OG	3:H:96:ILE:CA	2.55	0.54
3:H:99:HIS:HE2	5:U:270:GLY:C	2.15	0.54
3:H:166:PHE:CD1	4:L:176:SER:HB2	2.43	0.54
5:U:32:TRP:CE3	5:U:63:ILE:HD12	2.43	0.54
5:U:200:ASN:N	5:U:204:GLY:HA3	2.23	0.54
1:A:61:LYS:HB3	1:A:101:TYR:CZ	2.43	0.53
3:H:47:TRP:CD1	4:L:96:LEU:CD1	2.80	0.53
3:H:140:CYS:CB	3:H:179:SER:OG	2.46	0.53
5:U:60:GLY:O	5:U:62:LYS:N	2.41	0.53
5:U:73:LEU:O	5:U:74:ASP:C	2.51	0.53
5:U:137:ARG:CD	5:U:138:PRO:HD2	2.37	0.53
2:B:25:CYS:O	2:B:26:SER:C	2.51	0.53
3:H:33:TYR:HB2	3:H:96:ILE:CG1	2.38	0.53
5:U:55:LEU:C	5:U:55:LEU:CD2	2.80	0.53
5:U:190:ASN:ND2	5:U:215:CYS:CB	2.62	0.53
1:A:45:ASP:OD2	1:A:45:ASP:C	2.52	0.53
1:A:99:HIS:HD2	1:A:101:TYR:CA	2.18	0.53
2:B:8:ARG:C	2:B:10:THR:N	2.63	0.53
3:H:2:VAL:CG1	3:H:102:TYR:HD2	2.21	0.53
3:H:163:VAL:CG2	3:H:181:VAL:HG21	2.28	0.53
4:L:96:LEU:N	4:L:96:LEU:HD12	2.23	0.53
5:U:216:ARG:HH11	5:U:216:ARG:CG	2.17	0.53
1:A:20:VAL:HG23	1:A:20:VAL:O	2.09	0.53
1:A:43:GLU:C	1:A:44:ILE:HG13	2.33	0.53
1:A:55:GLY:O	1:A:56:HIS:C	2.51	0.53
3:H:105:GLN:CD	3:H:106:GLY:H	2.16	0.53
4:L:13:VAL:CG1	4:L:14:THR:N	2.72	0.53
1:A:43:GLU:C	1:A:44:ILE:CG1	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:TYR:CD2	3:H:98:GLY:N	2.64	0.53
1:A:44:ILE:N	1:A:44:ILE:CD1	2.53	0.53
3:H:145:TYR:C	3:H:174:LEU:CD2	2.82	0.53
4:L:185:GLU:C	4:L:185:GLU:CD	2.76	0.53
1:A:123:VAL:HG22	1:A:124:GLN:N	2.23	0.53
3:H:101:ASP:O	4:L:46:ARG:HB2	2.09	0.53
4:L:96:LEU:HD12	4:L:96:LEU:H	1.71	0.53
5:U:32:TRP:CH2	5:U:34:GLU:O	2.62	0.53
5:U:134:GLU:CG	5:U:135:GLU:N	2.72	0.53
1:A:58:TYR:CD2	1:A:58:TYR:O	2.62	0.53
3:H:33:TYR:HE2	3:H:97:TYR:CD1	2.27	0.53
3:H:145:TYR:CE1	3:H:150:VAL:CG2	2.90	0.53
4:L:142:LYS:HB3	4:L:173:TYR:CE1	2.44	0.53
3:H:152:VAL:CG1	3:H:196:ASN:O	2.57	0.53
4:L:27(A):SER:O	4:L:27(B):LEU:HD23	2.09	0.53
5:U:56:SER:N	5:U:147:CYS:O	2.41	0.53
5:U:195:TYR:HB2	5:U:272:ASN:CB	2.33	0.53
2:B:6:LYS:HG3	2:B:38:GLU:CG	2.38	0.52
3:H:105:GLN:HG2	3:H:106:GLY:N	2.23	0.52
4:L:192:TYR:CD2	4:L:209:PHE:HZ	2.22	0.52
5:U:2:ARG:HB2	5:U:74:ASP:OD2	2.09	0.52
5:U:6:CYS:N	5:U:43:LYS:O	2.34	0.52
5:U:52:ASN:OD1	5:U:70:VAL:N	2.39	0.52
1:A:112:TRP:HA	1:A:126:CYS:HB3	1.90	0.52
3:H:103:TRP:CD1	3:H:103:TRP:N	2.75	0.52
4:L:136:LEU:HB2	4:L:175:MET:HB3	1.90	0.52
5:U:116:ARG:N	5:U:120:GLU:OE2	2.42	0.52
3:H:47:TRP:CZ3	3:H:49:GLY:CA	2.84	0.52
3:H:60:ASN:O	3:H:63:ILE:HB	2.10	0.52
3:H:202:SER:O	3:H:203:SER:OG	2.21	0.52
4:L:35:TRP:CG	4:L:48:ILE:HD12	2.38	0.52
5:U:199:GLY:CA	5:U:236:TYR:HE1	2.22	0.52
1:A:54:ASN:OD1	1:A:56:HIS:N	2.43	0.52
3:H:105:GLN:CG	3:H:106:GLY:N	2.72	0.52
3:H:177:LEU:HD12	3:H:178:SER:N	2.24	0.52
4:L:117:ILE:CG2	4:L:133:VAL:O	2.58	0.52
5:U:211:PHE:O	5:U:213:ILE:HG23	2.08	0.52
5:U:268:LYS:O	5:U:269:SER:O	2.27	0.52
1:A:24:TYR:CG	5:U:150:LEU:HD13	2.45	0.52
1:A:35:LYS:C	1:A:37:PHE:H	2.17	0.52
1:A:64:THR:OG1	1:A:127:MET:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:32:TYR:C	3:H:96:ILE:HD13	2.34	0.52
3:H:51:ILE:HG13	3:H:52:ASN:N	2.24	0.52
4:L:120:PRO:HG2	4:L:186:TYR:HE2	1.74	0.52
3:H:22:CYS:HB3	3:H:78:ALA:HB3	1.92	0.52
3:H:33:TYR:CB	3:H:96:ILE:HG12	2.39	0.52
3:H:152:VAL:HG13	3:H:197:VAL:CG2	2.32	0.52
4:L:37:LEU:HD13	4:L:86:TYR:CE1	2.44	0.52
4:L:90:GLN:NE2	4:L:97:THR:H	2.08	0.52
4:L:185:GLU:HA	4:L:188:ARG:HG3	1.92	0.52
4:L:206:VAL:HG12	4:L:207:LYS:N	2.23	0.52
1:A:88:ARG:HH11	1:A:88:ARG:CG	2.21	0.52
2:B:27:TYR:HE2	5:U:116:ARG:CG	2.22	0.52
3:H:96:ILE:CG2	3:H:97:TYR:CA	2.84	0.52
4:L:146:VAL:HG21	4:L:161:ASN:ND2	2.25	0.52
4:L:164:THR:CB	4:L:174:SER:HB2	2.37	0.52
5:U:55:LEU:HA	5:U:148:GLY:HA3	1.92	0.52
5:U:123:LEU:HD12	5:U:146:GLY:O	2.08	0.52
1:A:59:ARG:HH11	1:A:94:LEU:C	2.18	0.52
3:H:38:LYS:O	3:H:45:LEU:HD23	2.10	0.52
4:L:49:TYR:O	4:L:50:LEU:HB2	2.07	0.52
5:U:229:HIS:CD2	5:U:230:GLU:N	2.75	0.52
1:A:22:ASN:O	1:A:27:ASN:HA	2.10	0.52
2:B:35:TYR:HD1	2:B:39:CYS:SG	2.33	0.52
4:L:164:THR:HG22	4:L:165:ASP:O	2.10	0.52
2:B:27:TYR:HE1	5:U:63:ILE:CG2	2.23	0.52
3:H:29:PHE:CD1	3:H:29:PHE:O	2.63	0.52
3:H:188:TRP:CD1	3:H:189:PRO:N	2.78	0.52
4:L:36:LEU:HG	4:L:36:LEU:O	2.09	0.52
5:U:195:TYR:N	5:U:272:ASN:HD22	2.08	0.52
1:A:52:GLU:O	1:A:53:GLY:C	2.53	0.51
3:H:100(B):LEU:N	3:H:100(B):LEU:CD1	2.71	0.51
5:U:270:GLY:C	5:U:272:ASN:H	2.17	0.51
3:H:52:ASN:OD1	3:H:52:ASN:C	2.52	0.51
3:H:105:GLN:OE1	3:H:105:GLN:N	2.42	0.51
3:H:124:LEU:HB2	3:H:139:GLY:HA3	1.91	0.51
4:L:43:SER:O	4:L:45:LYS:HE3	2.11	0.51
5:U:123:LEU:CB	5:U:169:LYS:O	2.57	0.51
5:U:195:TYR:HD1	5:U:210:THR:CG2	2.18	0.51
3:H:124:LEU:HB3	4:L:118:PHE:HD2	1.75	0.51
3:H:178:SER:CB	4:L:176:SER:OG	2.56	0.51
4:L:4:MET:HB2	4:L:98:PHE:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:36:LEU:HD12	4:L:45:LYS:O	2.11	0.51
5:U:133:GLY:HA2	5:U:137:ARG:NH2	2.26	0.51
2:B:24:LEU:O	2:B:24:LEU:HD22	2.10	0.51
3:H:47:TRP:HE1	4:L:96:LEU:HD13	1.63	0.51
4:L:187:GLU:OE1	4:L:211:ARG:NH2	2.44	0.51
5:U:153:CYS:N	5:U:154:PRO:CD	2.74	0.51
1:A:88:ARG:NH1	1:A:88:ARG:HG2	2.26	0.51
3:H:154:TRP:CE2	3:H:181:VAL:HG12	2.46	0.51
4:L:164:THR:CG2	4:L:165:ASP:N	2.73	0.51
5:U:25:ARG:CZ	5:U:44:SER:OG	2.59	0.51
1:A:23:LYS:N	5:U:140:ASP:OD1	2.38	0.51
3:H:29:PHE:C	3:H:29:PHE:CD1	2.86	0.51
4:L:148:TRP:CD2	4:L:179:LEU:CD2	2.77	0.51
2:B:25:CYS:HB2	2:B:31:CYS:N	2.26	0.51
3:H:101:ASP:CG	3:H:102:TYR:HD1	2.19	0.51
4:L:38:GLN:HA	4:L:44:PRO:HA	1.93	0.51
5:U:104:SER:O	5:U:109:ARG:HG3	2.10	0.51
5:U:184:LEU:CD1	5:U:216:ARG:CD	2.89	0.51
4:L:81:GLU:H	4:L:81:GLU:CD	2.18	0.51
4:L:148:TRP:NE1	4:L:179:LEU:HD22	2.26	0.51
5:U:117:SER:HG	5:U:118:PRO:HD2	1.73	0.51
5:U:136:GLY:O	5:U:137:ARG:HB2	2.11	0.51
1:A:35:LYS:C	1:A:37:PHE:N	2.68	0.51
1:A:43:GLU:C	1:A:44:ILE:CD1	2.84	0.51
1:A:69:ARG:HB2	1:A:70:PRO:CD	2.29	0.51
3:H:6:GLN:HE22	3:H:107:THR:HB	1.76	0.51
3:H:45:LEU:CD1	4:L:87:TYR:CE2	2.92	0.51
3:H:166:PHE:CE2	4:L:175:MET:CA	2.94	0.51
3:H:197:VAL:O	3:H:206:VAL:HG12	2.11	0.51
3:H:210:ILE:CG2	3:H:212:PRO:HD3	2.38	0.51
4:L:165:ASP:O	4:L:166:GLN:C	2.54	0.51
3:H:32:TYR:CB	3:H:96:ILE:HG21	2.40	0.50
4:L:140:TYR:HA	4:L:141:PRO:C	2.36	0.50
5:U:132:GLU:HG3	5:U:136:GLY:CA	2.40	0.50
5:U:190:ASN:HD21	5:U:216:ARG:N	2.08	0.50
1:A:51:TYR:CD2	1:A:130:ASP:HA	2.45	0.50
1:A:54:ASN:ND2	1:A:107:ASN:HA	2.25	0.50
3:H:47:TRP:HH2	3:H:58:SER:HB3	1.76	0.50
4:L:179:LEU:O	4:L:181:LEU:HD11	2.11	0.50
5:U:39:GLU:HA	5:U:40:LEU:CD2	2.42	0.50
3:H:47:TRP:HE3	3:H:60:ASN:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:32:TYR:N	4:L:32:TYR:CD2	2.78	0.50
4:L:89:TRP:CB	4:L:98:PHE:CD2	2.91	0.50
5:U:55:LEU:H	5:U:148:GLY:CA	2.25	0.50
5:U:234:GLN:O	5:U:235:SER:HB3	2.12	0.50
1:A:73:PRO:O	1:A:74:TRP:C	2.52	0.50
2:B:20:GLN:H	2:B:20:GLN:CD	2.14	0.50
2:B:35:TYR:O	2:B:36:THR:C	2.54	0.50
3:H:21:SER:CB	3:H:23:LYS:HZ2	2.24	0.50
4:L:83:LEU:HD23	4:L:83:LEU:C	2.37	0.50
4:L:86:TYR:HB2	4:L:102:THR:O	2.11	0.50
4:L:115:VAL:HG11	4:L:117:ILE:HD11	1.93	0.50
3:H:169:VAL:O	3:H:175:TYR:HA	2.11	0.50
3:H:35:HIS:HB2	3:H:100(B):LEU:HD21	1.94	0.50
4:L:85:VAL:O	4:L:86:TYR:HD1	1.93	0.50
4:L:139:PHE:N	4:L:139:PHE:CD1	2.79	0.50
5:U:39:GLU:HA	5:U:40:LEU:HD22	1.93	0.50
1:A:66:THR:HG22	1:A:67:MET:N	2.27	0.50
3:H:9:PRO:HB3	3:H:108:SER:CB	2.42	0.50
3:H:47:TRP:CE2	4:L:96:LEU:CD1	2.92	0.50
3:H:80:MET:HE3	3:H:82:PHE:CD1	2.47	0.50
3:H:82:PHE:HD2	3:H:82:PHE:C	2.20	0.50
3:H:124:LEU:CD1	4:L:133:VAL:HG23	2.42	0.50
5:U:4:MET:CE	5:U:78:GLN:CB	2.85	0.50
5:U:209:GLU:O	5:U:210:THR:C	2.52	0.50
1:A:12:ASP:OD2	1:A:12:ASP:N	2.45	0.50
3:H:101:ASP:HA	4:L:46:ARG:CD	2.32	0.50
3:H:135:MET:C	3:H:136:VAL:HG13	2.37	0.50
3:H:145:TYR:CD1	3:H:150:VAL:HG21	2.46	0.50
4:L:151:ASP:OD2	4:L:189:HIS:CD2	2.64	0.50
5:U:192:ARG:HD3	5:U:269:SER:OG	2.11	0.50
1:A:44:ILE:HG23	1:A:59:ARG:CB	2.42	0.49
1:A:116:GLN:OE1	1:A:119:LEU:O	2.30	0.49
4:L:33:LEU:HD12	4:L:71:PHE:CD2	2.47	0.49
5:U:9:ASN:OD1	5:U:11:ASP:N	2.45	0.49
5:U:195:TYR:C	5:U:272:ASN:HD22	2.19	0.49
1:A:112:TRP:HZ3	1:A:114:TYR:CE1	2.30	0.49
4:L:10:THR:HG23	4:L:10:THR:O	2.11	0.49
5:U:99:GLY:H	5:U:104:SER:CB	2.08	0.49
4:L:159:VAL:HG12	4:L:161:ASN:OD1	2.12	0.49
1:A:33:CYS:HB3	1:A:34:PRO:HD2	1.94	0.49
3:H:122:TYR:CD1	4:L:124:GLN:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:142:VAL:CG2	3:H:177:LEU:CD1	2.88	0.49
4:L:27(B):LEU:HD13	4:L:90:GLN:HB3	1.93	0.49
4:L:94:PHE:N	4:L:94:PHE:HD2	2.11	0.49
1:A:87:HIS:CE1	5:U:11:ASP:CA	2.88	0.49
3:H:20:ILE:HD12	3:H:107:THR:HG21	1.94	0.49
3:H:105:GLN:NE2	3:H:106:GLY:O	2.45	0.49
3:H:155:ASN:ND2	3:H:194:THR:H	2.11	0.49
4:L:37:LEU:HD13	4:L:85:VAL:O	2.10	0.49
4:L:138:ASN:ND2	4:L:170:ASP:CG	2.70	0.49
2:B:2:GLN:OE1	2:B:4:SER:CB	2.60	0.49
3:H:6:GLN:CG	3:H:105:GLN:NE2	2.73	0.49
5:U:264:SER:C	5:U:265:CYS:SG	2.96	0.49
1:A:22:ASN:HD22	5:U:66:LEU:HD12	1.73	0.49
1:A:112:TRP:CD1	1:A:112:TRP:N	2.81	0.49
3:H:101:ASP:CG	3:H:102:TYR:N	2.70	0.49
4:L:32:TYR:O	4:L:34:ASN:CG	2.56	0.49
4:L:186:TYR:HD1	4:L:186:TYR:O	1.95	0.49
5:U:193:GLN:H	5:U:269:SER:CB	2.26	0.49
4:L:44:PRO:C	4:L:45:LYS:HG2	2.37	0.49
5:U:34:GLU:HG3	5:U:35:GLY:H	1.78	0.49
5:U:141:ASP:HB3	5:U:143:HIS:O	2.13	0.49
1:A:34:PRO:HB2	1:A:35:LYS:CE	2.40	0.49
1:A:63:SER:CB	1:A:100:ASN:ND2	2.75	0.49
1:A:110:ARG:NH2	1:A:126:CYS:O	2.45	0.49
3:H:60:ASN:O	3:H:61:GLN:C	2.55	0.49
3:H:101:ASP:CB	3:H:102:TYR:HD1	2.25	0.49
4:L:25:SER:HB3	4:L:27(B):LEU:HD11	1.93	0.49
1:A:88:ARG:NH1	1:A:90:ASP:OD1	2.45	0.49
3:H:59:TYR:HH	3:H:68:THR:HA	1.75	0.49
4:L:27(B):LEU:O	4:L:31:THR:CG2	2.58	0.49
5:U:184:LEU:C	5:U:184:LEU:CD1	2.86	0.49
1:A:88:ARG:HB3	1:A:90:ASP:OD1	2.13	0.48
4:L:40:PRO:HD3	4:L:84:GLY:CA	2.43	0.48
5:U:59:THR:CG2	5:U:101:SER:HB2	2.43	0.48
5:U:185:GLU:HG3	5:U:186:ASN:N	2.27	0.48
3:H:31:SER:O	5:U:212:LEU:HD13	2.12	0.48
3:H:124:LEU:HD12	4:L:133:VAL:CG2	2.42	0.48
3:H:154:TRP:HZ3	3:H:195:CYS:CB	1.99	0.48
3:H:169:VAL:HG12	3:H:170:LEU:N	2.27	0.48
1:A:41:HIS:O	1:A:42:CYS:SG	2.71	0.48
1:A:110:ARG:C	1:A:111:PRO:O	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:CYS:O	2:B:7:GLY:N	2.46	0.48
3:H:29:PHE:CD2	3:H:76:ARG:HA	2.46	0.48
3:H:168:ALA:HA	3:H:177:LEU:HB3	1.94	0.48
4:L:85:VAL:C	4:L:86:TYR:HD1	2.21	0.48
4:L:155:ARG:HB2	4:L:155:ARG:CZ	2.42	0.48
5:U:40:LEU:CD2	5:U:40:LEU:N	2.65	0.48
5:U:66:LEU:O	5:U:67:THR:CB	2.60	0.48
5:U:184:LEU:HA	5:U:187:LEU:HD13	1.94	0.48
3:H:36:TRP:CE3	3:H:92:CYS:HB3	2.47	0.48
3:H:100:SER:C	3:H:100(A):VAL:HG13	2.38	0.48
3:H:101:ASP:HB2	3:H:102:TYR:CD1	2.48	0.48
3:H:101:ASP:HB2	3:H:102:TYR:HD1	1.77	0.48
3:H:148:GLU:HB3	3:H:149:PRO:HA	1.94	0.48
4:L:4:MET:CB	4:L:99:GLY:HA2	2.43	0.48
5:U:2:ARG:O	5:U:3:CYS:SG	2.71	0.48
5:U:61:LEU:N	5:U:61:LEU:CD1	2.47	0.48
5:U:202:THR:O	5:U:203:HIS:CG	2.66	0.48
5:U:205:CYS:SG	5:U:237:MET:CE	3.02	0.48
1:A:15:ASN:ND2	1:A:37:PHE:CZ	2.79	0.48
2:B:27:TYR:CE1	5:U:63:ILE:CG2	2.95	0.48
4:L:139:PHE:CZ	4:L:175:MET:HB2	2.47	0.48
5:U:229:HIS:C	5:U:230:GLU:O	2.56	0.48
1:A:44:ILE:HG22	1:A:60:GLY:CA	2.43	0.48
1:A:59:ARG:HB3	1:A:103:ARG:CZ	2.43	0.48
3:H:100(A):VAL:CA	4:L:89:TRP:HH2	2.26	0.48
3:H:5:GLN:O	3:H:23:LYS:HG2	2.14	0.48
5:U:28:ILE:HD12	5:U:28:ILE:N	2.22	0.48
5:U:113:LEU:O	5:U:113:LEU:CD2	2.52	0.48
1:A:41:HIS:HB2	1:A:43:GLU:HG2	1.95	0.48
1:A:51:TYR:CD2	1:A:129:HIS:O	2.67	0.48
2:B:22:ASP:OD1	2:B:24:LEU:CA	2.62	0.48
3:H:199:HIS:HE1	3:H:201:ALA:CB	2.13	0.48
4:L:89:TRP:HB2	4:L:97:THR:O	2.14	0.48
4:L:150:ILE:HG22	4:L:189:HIS:CD2	2.48	0.48
5:U:25:ARG:NE	5:U:44:SER:OG	2.46	0.48
3:H:41:HIS:ND1	3:H:44:SER:HB2	2.29	0.48
3:H:145:TYR:N	3:H:174:LEU:HD22	2.28	0.48
4:L:65:SER:OG	4:L:66:GLY:N	2.42	0.48
4:L:185:GLU:O	4:L:186:TYR:C	2.57	0.48
5:U:184:LEU:C	5:U:184:LEU:HD12	2.39	0.48
1:A:53:GLY:O	1:A:54:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:HE1	1:A:103:ARG:HG2	1.78	0.48
1:A:91:ALA:C	1:A:93:GLN:N	2.71	0.48
1:A:103:ARG:O	1:A:112:TRP:N	2.45	0.48
3:H:62:LYS:O	3:H:63:ILE:C	2.56	0.48
3:H:135:MET:C	3:H:136:VAL:CG1	2.87	0.48
3:H:166:PHE:HA	3:H:167:PRO:HD3	1.51	0.48
4:L:1:ASP:OD2	4:L:95:PRO:HG3	2.14	0.48
4:L:59:PRO:CG	4:L:62:PHE:HE1	2.24	0.48
5:U:102:ASP:CG	5:U:104:SER:HB2	2.39	0.48
5:U:190:ASN:OD1	5:U:215:CYS:HB2	2.13	0.48
5:U:193:GLN:H	5:U:269:SER:HB3	1.78	0.48
1:A:54:ASN:O	1:A:54:ASN:CG	2.57	0.47
3:H:50:GLU:HG2	3:H:58:SER:CB	2.44	0.47
3:H:170:LEU:O	3:H:171:GLN:HB2	2.13	0.47
4:L:15:ILE:C	4:L:17:GLN:H	2.22	0.47
5:U:184:LEU:HD11	5:U:216:ARG:CD	2.44	0.47
5:U:198:LYS:O	5:U:204:GLY:C	2.57	0.47
7:U:303:MAN:O2	6:C:2:NAG:H62	2.14	0.47
1:A:85:HIS:HD2	1:A:87:HIS:N	1.97	0.47
1:A:106:ASP:OD2	1:A:108:ARG:CG	2.62	0.47
3:H:94:ARG:CA	3:H:96:ILE:HD12	2.43	0.47
3:H:97:TYR:O	3:H:98:GLY:C	2.57	0.47
3:H:136:VAL:N	3:H:183:VAL:O	2.46	0.47
4:L:115:VAL:HG12	4:L:116:SER:N	2.29	0.47
1:A:56:HIS:CG	1:A:57:PHE:CE1	3.03	0.47
3:H:26:GLY:O	3:H:27:TYR:HB3	2.13	0.47
3:H:43:LYS:HZ3	3:H:43:LYS:C	2.21	0.47
4:L:89:TRP:CB	4:L:98:PHE:HD2	2.24	0.47
4:L:111:ALA:O	4:L:198:HIS:CE1	2.68	0.47
1:A:26:SER:OG	5:U:25:ARG:CZ	2.63	0.47
1:A:51:TYR:HD1	1:A:111:PRO:HD3	1.79	0.47
3:H:154:TRP:NE1	3:H:181:VAL:CG1	2.78	0.47
3:H:155:ASN:OD1	3:H:193:VAL:HG22	2.14	0.47
4:L:62:PHE:HA	4:L:74:LYS:O	2.13	0.47
5:U:59:THR:CG2	5:U:101:SER:CB	2.91	0.47
5:U:94:GLU:HG2	5:U:175:LYS:HD3	1.96	0.47
3:H:82:PHE:C	3:H:82:PHE:CD2	2.92	0.47
3:H:144:GLY:O	3:H:174:LEU:CD2	2.62	0.47
3:H:190:SER:OG	3:H:191:GLN:HG2	2.14	0.47
4:L:206:VAL:CG1	4:L:207:LYS:N	2.78	0.47
5:U:123:LEU:CA	5:U:169:LYS:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:165:PHE:CD1	5:U:184:LEU:HB2	2.50	0.47
1:A:40:GLN:CD	5:U:8:THR:CG2	2.88	0.47
2:B:13:PHE:CD1	2:B:14:ASN:N	2.82	0.47
3:H:12:VAL:O	3:H:111:VAL:CG1	2.62	0.47
3:H:122:TYR:CD2	4:L:124:GLN:HB2	2.50	0.47
3:H:184:PRO:HB2	3:H:187:THR:OG1	2.14	0.47
3:H:192:THR:CG2	3:H:209:LYS:NZ	2.76	0.47
4:L:150:ILE:CG2	4:L:189:HIS:CD2	2.97	0.47
5:U:126:VAL:HB	5:U:167:PHE:HB3	1.95	0.47
5:U:163:ASP:OD1	5:U:164:THR:HB	2.15	0.47
5:U:184:LEU:HD12	5:U:216:ARG:HD3	1.95	0.47
5:U:221:GLN:O	5:U:242:ALA:N	2.40	0.47
1:A:120:LYS:HA	1:A:121:PRO:HD2	1.75	0.47
2:B:25:CYS:O	2:B:28:TYR:N	2.44	0.47
3:H:53:TYR:CE2	5:U:214:ASP:CG	2.92	0.47
3:H:166:PHE:HE2	4:L:175:MET:N	2.12	0.47
4:L:136:LEU:HD13	4:L:144:ILE:CD1	2.44	0.47
5:U:69:VAL:CG2	5:U:70:VAL:N	2.77	0.47
5:U:102:ASP:O	5:U:103:MET:HB2	2.15	0.47
5:U:129:TRP:HE1	5:U:138:PRO:HG2	1.75	0.47
1:A:36:LYS:C	1:A:37:PHE:CD2	2.92	0.47
4:L:183:LYS:O	4:L:184:ASP:C	2.57	0.47
4:L:186:TYR:O	4:L:186:TYR:CD1	2.68	0.47
5:U:32:TRP:CD2	5:U:63:ILE:HD12	2.50	0.47
5:U:274:PRO:O	5:U:275:ASP:CB	2.62	0.47
4:L:136:LEU:HD12	4:L:175:MET:CG	2.45	0.47
5:U:3:CYS:N	5:U:75:LEU:HD23	2.30	0.47
1:A:102:CYS:O	1:A:103:ARG:HD3	2.14	0.47
3:H:45:LEU:HD23	3:H:45:LEU:HA	1.61	0.47
4:L:27(D):ASP:C	4:L:28:ASP:H	2.21	0.47
4:L:118:PHE:CD1	4:L:118:PHE:N	2.80	0.47
5:U:157:ASN:O	5:U:168:LEU:N	2.46	0.47
5:U:223:LEU:C	5:U:224:VAL:HG23	2.40	0.47
1:A:51:TYR:HD1	1:A:111:PRO:CD	2.27	0.46
2:B:34:ASP:OD2	2:B:34:ASP:C	2.58	0.46
3:H:152:VAL:HG13	3:H:196:ASN:O	2.15	0.46
3:H:47:TRP:CE3	3:H:60:ASN:HB2	2.50	0.46
3:H:123:PRO:HD2	4:L:121:SER:OG	2.15	0.46
5:U:190:ASN:ND2	5:U:216:ARG:N	2.62	0.46
5:U:236:TYR:CG	5:U:237:MET:N	2.83	0.46
1:A:29:HIS:N	1:A:29:HIS:ND1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:52:SER:OG	4:L:53:LYS:N	2.48	0.46
4:L:148:TRP:CD1	4:L:179:LEU:HD13	2.50	0.46
5:U:9:ASN:OD1	5:U:10:GLY:C	2.59	0.46
1:A:69:ARG:HH11	1:A:115:VAL:HG11	1.79	0.46
2:B:6:LYS:CD	2:B:38:GLU:CD	2.88	0.46
3:H:97:TYR:HE2	5:U:212:LEU:HD22	1.79	0.46
4:L:90:GLN:NE2	4:L:97:THR:N	2.64	0.46
4:L:122:SER:OG	4:L:123:GLU:N	2.48	0.46
5:U:187:LEU:CB	5:U:188:PRO:CD	2.93	0.46
2:B:13:PHE:HE1	2:B:20:GLN:CD	2.22	0.46
3:H:60:ASN:ND2	4:L:95:PRO:HB2	2.30	0.46
3:H:142:VAL:CG2	3:H:177:LEU:HG	2.45	0.46
4:L:15:ILE:HD12	4:L:79:GLU:HA	1.98	0.46
5:U:123:LEU:HD12	5:U:123:LEU:H	1.79	0.46
5:U:157:ASN:CB	5:U:245:SER:HB3	2.45	0.46
1:A:119:LEU:HA	1:A:119:LEU:HD22	1.39	0.46
4:L:90:GLN:HE21	4:L:97:THR:N	2.14	0.46
4:L:155:ARG:HG3	4:L:157:ASN:H	1.80	0.46
4:L:170:ASP:C	4:L:172:THR:N	2.73	0.46
5:U:1:LEU:C	5:U:2:ARG:HG3	2.40	0.46
5:U:97:SER:OG	5:U:145:ARG:O	2.27	0.46
1:A:22:ASN:HA	5:U:140:ASP:OD1	2.15	0.46
1:A:123:VAL:CG2	1:A:124:GLN:N	2.78	0.46
3:H:146:PHE:CD2	3:H:147:PRO:CA	2.96	0.46
4:L:46:ARG:NH2	4:L:49:TYR:HE1	2.13	0.46
4:L:112:ALA:HA	4:L:113:PRO:HD2	1.73	0.46
4:L:180:THR:O	4:L:181:LEU:HD23	2.15	0.46
5:U:137:ARG:HD3	5:U:138:PRO:CD	2.42	0.46
5:U:190:ASN:OD1	5:U:215:CYS:O	2.34	0.46
1:A:80:LEU:CD2	1:A:85:HIS:CD2	2.95	0.46
4:L:38:GLN:HG3	4:L:44:PRO:CB	2.46	0.46
4:L:51:VAL:O	4:L:51:VAL:HG12	2.15	0.46
4:L:83:LEU:CD1	4:L:167:ASP:O	2.63	0.46
4:L:191:SER:CB	4:L:210:ASN:HD21	2.12	0.46
5:U:97:SER:HB2	5:U:146:GLY:CA	2.46	0.46
5:U:216:ARG:O	5:U:219:MET:HE3	2.15	0.46
5:U:238:VAL:CG1	5:U:239:ARG:N	2.79	0.46
1:A:74:TRP:CH2	1:A:113:CYS:HA	2.50	0.46
2:B:25:CYS:HB2	2:B:31:CYS:CA	2.46	0.46
3:H:97:TYR:CD2	5:U:212:LEU:CD2	2.94	0.46
4:L:37:LEU:CD1	4:L:38:GLN:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:54:LEU:HD23	4:L:54:LEU:HA	1.43	0.46
1:A:44:ILE:HD12	1:A:44:ILE:H	1.76	0.46
1:A:61:LYS:HG2	1:A:101:TYR:CZ	2.51	0.46
2:B:25:CYS:HB2	2:B:31:CYS:HA	1.98	0.46
3:H:75:SER:OG	3:H:77:THR:HB	2.16	0.46
3:H:170:LEU:CD1	3:H:174:LEU:O	2.63	0.46
4:L:13:VAL:CG1	4:L:14:THR:H	2.28	0.46
4:L:49:TYR:HD2	4:L:50:LEU:HB2	1.81	0.46
4:L:90:GLN:HE21	4:L:97:THR:H	1.63	0.46
5:U:52:ASN:OD1	5:U:69:VAL:CA	2.63	0.46
5:U:99:GLY:O	5:U:104:SER:CA	2.65	0.46
5:U:159:PHE:HZ	5:U:161:ASN:ND2	2.14	0.46
1:A:110:ARG:O	1:A:111:PRO:O	2.34	0.45
3:H:20:ILE:O	3:H:20:ILE:HG13	2.06	0.45
4:L:4:MET:HB3	4:L:99:GLY:HA2	1.98	0.45
4:L:61:ARG:NH2	4:L:79:GLU:OE1	2.49	0.45
4:L:68:GLY:O	4:L:71:PHE:HE1	1.99	0.45
3:H:146:PHE:HB2	3:H:174:LEU:HA	1.99	0.45
3:H:167:PRO:CD	4:L:162:SER:OG	2.63	0.45
4:L:161:ASN:HB3	4:L:175:MET:HE3	1.95	0.45
5:U:59:THR:HG22	5:U:101:SER:HB2	1.97	0.45
5:U:194:CYS:SG	5:U:241:CYS:SG	3.14	0.45
2:B:15:VAL:O	2:B:15:VAL:HG22	2.17	0.45
3:H:18:VAL:HG23	3:H:19:LYS:N	2.31	0.45
3:H:35:HIS:CB	3:H:100(B):LEU:HD21	2.45	0.45
3:H:50:GLU:H	3:H:58:SER:HB2	1.82	0.45
3:H:136:VAL:CG2	3:H:183:VAL:HG23	2.46	0.45
4:L:27(D):ASP:O	4:L:28:ASP:N	2.50	0.45
5:U:18:ALA:C	5:U:19:LEU:HD12	2.42	0.45
5:U:123:LEU:N	5:U:123:LEU:CD1	2.69	0.45
5:U:132:GLU:HG3	5:U:136:GLY:HA2	1.98	0.45
3:H:187:THR:O	3:H:187:THR:HG22	2.15	0.45
4:L:13:VAL:HG12	4:L:14:THR:H	1.80	0.45
4:L:78:VAL:C	4:L:79:GLU:HG3	2.41	0.45
4:L:116:SER:HB3	4:L:118:PHE:HE1	1.76	0.45
4:L:136:LEU:O	4:L:175:MET:N	2.50	0.45
4:L:139:PHE:CE1	4:L:175:MET:HB2	2.51	0.45
5:U:32:TRP:CZ3	5:U:34:GLU:N	2.84	0.45
5:U:204:GLY:O	5:U:209:GLU:OE2	2.35	0.45
5:U:239:ARG:NH1	5:U:274:PRO:HB3	2.31	0.45
1:A:34:PRO:CA	1:A:35:LYS:HD3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLY:O	1:A:40:GLN:C	2.59	0.45
3:H:139:GLY:N	4:L:118:PHE:HE2	2.15	0.45
4:L:115:VAL:CG1	4:L:116:SER:N	2.79	0.45
4:L:166:GLN:HB2	4:L:173:TYR:CZ	2.52	0.45
5:U:118:PRO:CG	5:U:119:GLU:OE2	2.64	0.45
3:H:9:PRO:HB3	3:H:108:SER:HB3	1.99	0.45
3:H:60:ASN:ND2	4:L:95:PRO:CB	2.80	0.45
3:H:142:VAL:HG21	3:H:177:LEU:HD11	1.99	0.45
4:L:115:VAL:CG1	4:L:117:ILE:CD1	2.94	0.45
4:L:179:LEU:HA	4:L:179:LEU:HD12	1.44	0.45
5:U:28:ILE:CG2	5:U:29:VAL:N	2.74	0.45
5:U:99:GLY:O	5:U:104:SER:CB	2.64	0.45
5:U:117:SER:O	5:U:120:GLU:HB2	2.17	0.45
5:U:230:GLU:CB	5:U:231:PRO:CD	2.93	0.45
3:H:4:LEU:HB3	3:H:104:GLY:HA2	1.96	0.45
3:H:12:VAL:HB	3:H:111:VAL:CG1	2.45	0.45
3:H:144:GLY:C	3:H:174:LEU:CD1	2.89	0.45
1:A:94:LEU:HD22	1:A:105:PRO:HB3	1.99	0.45
2:B:6:LYS:HE3	2:B:38:GLU:CD	2.38	0.45
3:H:21:SER:HB2	3:H:23:LYS:HZ2	1.71	0.45
3:H:33:TYR:CE1	3:H:98:GLY:HA2	2.49	0.45
3:H:39:GLN:HA	3:H:45:LEU:HD23	1.97	0.45
3:H:51:ILE:HG13	3:H:52:ASN:H	1.81	0.45
4:L:32:TYR:O	4:L:34:ASN:ND2	2.49	0.45
5:U:66:LEU:O	5:U:67:THR:HG22	2.17	0.45
3:H:13:LYS:CE	3:H:113:SER:O	2.65	0.45
4:L:3:VAL:O	4:L:3:VAL:HG23	2.16	0.45
5:U:250:ALA:HB1	5:U:253:GLY:H	1.81	0.45
4:L:15:ILE:C	4:L:17:GLN:N	2.75	0.44
4:L:37:LEU:CG	4:L:38:GLN:N	2.77	0.44
5:U:219:MET:HB3	5:U:242:ALA:N	2.31	0.44
5:U:161:ASN:C	5:U:161:ASN:OD1	2.60	0.44
2:B:32:CYS:O	2:B:34:ASP:N	2.51	0.44
3:H:58:SER:C	3:H:59:TYR:CD1	2.83	0.44
3:H:101:ASP:OD2	3:H:102:TYR:CD1	2.70	0.44
5:U:25:ARG:NH1	5:U:27:THR:OG1	2.41	0.44
1:A:79:VAL:HG13	1:A:114:TYR:HE2	1.77	0.44
3:H:7:SER:OG	3:H:8:GLY:O	2.24	0.44
3:H:72:ASP:CG	3:H:75:SER:OG	2.60	0.44
3:H:118:PRO:HB3	3:H:202:SER:OG	2.17	0.44
3:H:149:PRO:O	3:H:150:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:63:THR:N	4:L:74:LYS:O	2.48	0.44
4:L:70:ASP:C	4:L:71:PHE:HD1	2.22	0.44
4:L:90:GLN:CD	4:L:90:GLN:C	2.86	0.44
5:U:66:LEU:O	5:U:67:THR:HB	2.18	0.44
5:U:134:GLU:HG2	5:U:135:GLU:HG2	1.99	0.44
5:U:223:LEU:O	5:U:224:VAL:CG2	2.65	0.44
3:H:29:PHE:O	3:H:31:SER:N	2.50	0.44
3:H:123:PRO:HD2	4:L:121:SER:HB3	1.98	0.44
1:A:83:THR:HG22	1:A:84:TYR:H	1.83	0.44
3:H:43:LYS:CE	3:H:43:LYS:CA	2.95	0.44
3:H:144:GLY:O	3:H:174:LEU:CD1	2.66	0.44
5:U:38:LEU:CD1	5:U:38:LEU:C	2.64	0.44
5:U:74:ASP:C	5:U:75:LEU:HG	2.43	0.44
5:U:137:ARG:HH22	5:U:198:LYS:HZ1	1.63	0.44
5:U:211:PHE:N	5:U:211:PHE:CD1	2.85	0.44
5:U:228:THR:HB	5:U:234:GLN:OE1	2.18	0.44
1:A:87:HIS:CD2	5:U:9:ASN:OD1	2.70	0.44
1:A:115:VAL:HG23	1:A:124:GLN:HB2	1.91	0.44
2:B:35:TYR:C	2:B:37:ALA:N	2.73	0.44
3:H:121:VAL:HG22	3:H:142:VAL:HA	2.00	0.44
3:H:184:PRO:CD	3:H:187:THR:OG1	2.66	0.44
4:L:55:ASP:HB3	4:L:58:VAL:HG23	1.99	0.44
4:L:90:GLN:HG3	4:L:97:THR:HG1	1.82	0.44
4:L:110:ASP:OD1	4:L:141:PRO:HD3	2.18	0.44
5:U:48:SER:OG	5:U:260:HIS:CE1	2.70	0.44
5:U:202:THR:C	5:U:204:GLY:H	2.24	0.44
3:H:100(B):LEU:N	4:L:89:TRP:CH2	2.85	0.44
4:L:27(D):ASP:C	4:L:28:ASP:N	2.76	0.44
5:U:30:ARG:C	5:U:31:LEU:HD22	2.35	0.44
5:U:223:LEU:HD23	5:U:224:VAL:CA	2.48	0.44
3:H:16:ALA:O	3:H:82(C):LEU:HD22	2.18	0.44
4:L:46:ARG:CD	4:L:49:TYR:HD1	2.24	0.44
5:U:89:ARG:HB2	5:U:92:TYR:OH	2.18	0.44
3:H:142:VAL:CG2	3:H:177:LEU:CG	2.96	0.43
4:L:33:LEU:CD1	4:L:51:VAL:HG22	2.43	0.43
4:L:140:TYR:CD1	4:L:141:PRO:HA	2.52	0.43
5:U:225:ALA:C	5:U:226:THR:HG23	2.43	0.43
5:U:228:THR:HB	5:U:234:GLN:HG2	2.00	0.43
2:B:34:ASP:O	2:B:37:ALA:CB	2.58	0.43
3:H:97:TYR:CD2	5:U:212:LEU:CD1	2.97	0.43
3:H:100(B):LEU:H	3:H:100(B):LEU:CD1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:170:LEU:HD12	3:H:174:LEU:O	2.17	0.43
4:L:46:ARG:NH1	4:L:49:TYR:CD1	2.86	0.43
4:L:150:ILE:O	4:L:153:SER:N	2.48	0.43
5:U:39:GLU:HG3	5:U:40:LEU:N	2.33	0.43
1:A:25:PHE:CE2	5:U:66:LEU:HB3	2.54	0.43
1:A:103:ARG:HD3	1:A:103:ARG:HA	1.73	0.43
3:H:13:LYS:HD3	3:H:13:LYS:HA	1.80	0.43
4:L:67:SER:O	4:L:70:ASP:O	2.35	0.43
4:L:83:LEU:HB2	4:L:106:LEU:HD21	2.00	0.43
4:L:122:SER:O	4:L:125:LEU:N	2.49	0.43
5:U:58:ARG:HB2	5:U:113:LEU:CD1	2.48	0.43
1:A:56:HIS:CB	1:A:57:PHE:HD1	2.04	0.43
2:B:6:LYS:CB	2:B:38:GLU:HG3	2.48	0.43
3:H:6:GLN:NE2	3:H:107:THR:OG1	2.51	0.43
4:L:48:ILE:HG22	4:L:49:TYR:N	2.33	0.43
5:U:3:CYS:N	5:U:75:LEU:CD2	2.81	0.43
5:U:107:ARG:HB2	5:U:109:ARG:HD2	1.99	0.43
1:A:105:PRO:O	1:A:105:PRO:HG2	2.18	0.43
2:B:35:TYR:CD1	2:B:39:CYS:SG	3.12	0.43
4:L:122:SER:O	4:L:125:LEU:HB2	2.19	0.43
5:U:195:TYR:CD1	5:U:210:THR:HG22	2.38	0.43
1:A:34:PRO:C	1:A:35:LYS:HD3	2.43	0.43
3:H:9:PRO:HB3	3:H:108:SER:OG	2.19	0.43
3:H:60:ASN:OD1	3:H:61:GLN:N	2.52	0.43
4:L:21:ILE:HG13	4:L:73:LEU:HD23	2.01	0.43
4:L:51:VAL:CG2	4:L:71:PHE:CE2	3.00	0.43
4:L:90:GLN:CG	4:L:97:THR:OG1	2.66	0.43
4:L:133:VAL:HG12	4:L:134:CYS:N	2.33	0.43
5:U:29:VAL:CG1	5:U:66:LEU:HD23	2.45	0.43
5:U:125:VAL:O	5:U:125:VAL:CG1	2.62	0.43
1:A:61:LYS:CA	1:A:101:TYR:CG	2.86	0.43
1:A:73:PRO:CG	1:A:76:SER:HB3	2.49	0.43
2:B:31:CYS:SG	2:B:35:TYR:HD2	2.40	0.43
3:H:16:ALA:O	3:H:82(C):LEU:CD2	2.67	0.43
3:H:47:TRP:CH2	3:H:49:GLY:C	2.96	0.43
3:H:77:THR:HG23	3:H:78:ALA:O	2.19	0.43
4:L:51:VAL:HG21	4:L:71:PHE:CE2	2.41	0.43
4:L:170:ASP:HB2	4:L:172:THR:OG1	2.19	0.43
5:U:52:ASN:ND2	5:U:69:VAL:HG23	2.34	0.43
5:U:239:ARG:HH22	5:U:274:PRO:CA	2.12	0.43
1:A:85:HIS:HD2	1:A:86:ALA:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:CG	2:B:14:ASN:N	2.86	0.43
2:B:36:THR:O	2:B:39:CYS:O	2.37	0.43
3:H:95:SER:H	3:H:96:ILE:HD11	1.71	0.43
3:H:142:VAL:CB	3:H:177:LEU:HG	2.47	0.43
3:H:148:GLU:CB	3:H:149:PRO:HA	2.48	0.43
5:U:95:CYS:C	5:U:96:ILE:HD13	2.43	0.43
5:U:29:VAL:CG1	5:U:66:LEU:CD2	2.77	0.43
1:A:74:TRP:CG	1:A:96:LEU:HD13	2.54	0.42
3:H:2:VAL:CB	3:H:102:TYR:HD2	2.32	0.42
3:H:102:TYR:C	3:H:103:TRP:CD1	2.97	0.42
3:H:143:LYS:HG2	3:H:144:GLY:H	1.83	0.42
4:L:24:LYS:N	4:L:24:LYS:CD	2.80	0.42
4:L:46:ARG:CZ	4:L:49:TYR:CD1	3.02	0.42
5:U:118:PRO:CD	5:U:119:GLU:OE2	2.67	0.42
5:U:273:HIS:C	5:U:275:ASP:N	2.77	0.42
1:A:11:CYS:C	1:A:12:ASP:OD2	2.62	0.42
3:H:18:VAL:CG2	3:H:19:LYS:N	2.78	0.42
3:H:94:ARG:O	3:H:100(B):LEU:CA	2.62	0.42
4:L:32:TYR:HD1	4:L:91:GLY:O	2.03	0.42
4:L:148:TRP:HE1	4:L:179:LEU:HD13	1.79	0.42
4:L:179:LEU:C	4:L:181:LEU:HD11	2.44	0.42
5:U:184:LEU:HD11	5:U:216:ARG:HD2	2.01	0.42
3:H:97:TYR:HD2	5:U:212:LEU:CD1	2.24	0.42
4:L:62:PHE:CD1	4:L:62:PHE:N	2.87	0.42
5:U:23:LEU:HA	5:U:23:LEU:HD23	1.65	0.42
5:U:129:TRP:CE2	5:U:138:PRO:CG	3.00	0.42
1:A:13:CYS:SG	1:A:19:CYS:CB	2.98	0.42
1:A:14:LEU:HB2	1:A:15:ASN:OD1	2.19	0.42
1:A:43:GLU:H	1:A:43:GLU:HG3	1.33	0.42
1:A:94:LEU:HD13	1:A:105:PRO:HB3	1.98	0.42
3:H:95:SER:HB3	3:H:96:ILE:HA	1.97	0.42
5:U:133:GLY:N	5:U:137:ARG:CG	2.68	0.42
1:A:39:GLY:O	1:A:42:CYS:N	2.29	0.42
1:A:58:TYR:O	1:A:58:TYR:CG	2.69	0.42
2:B:13:PHE:CE1	2:B:20:GLN:CD	2.97	0.42
4:L:132:VAL:HG12	4:L:148:TRP:CH2	2.54	0.42
5:U:161:ASN:HB2	5:U:196:SER:CB	2.48	0.42
3:H:60:ASN:O	3:H:63:ILE:CB	2.68	0.42
3:H:63:ILE:HG22	3:H:65:GLY:CA	2.43	0.42
3:H:96:ILE:CG2	3:H:97:TYR:N	2.82	0.42
3:H:102:TYR:N	3:H:102:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:145:TYR:CE1	3:H:150:VAL:HG21	2.55	0.42
3:H:152:VAL:HG12	3:H:196:ASN:O	2.19	0.42
4:L:13:VAL:HG11	4:L:78:VAL:HG21	2.02	0.42
4:L:151:ASP:OD2	4:L:189:HIS:CG	2.73	0.42
4:L:180:THR:C	4:L:181:LEU:CD2	2.93	0.42
5:U:21:GLN:HB3	5:U:47:HIS:HA	2.00	0.42
5:U:95:CYS:O	5:U:96:ILE:HD13	2.18	0.42
1:A:37:PHE:N	1:A:37:PHE:CD2	2.88	0.42
1:A:61:LYS:O	1:A:62:ALA:CB	2.67	0.42
4:L:120:PRO:HD2	4:L:186:TYR:HE2	1.83	0.42
5:U:27:THR:O	5:U:28:ILE:CD1	2.37	0.42
5:U:39:GLU:O	5:U:40:LEU:HD22	2.04	0.42
5:U:96:ILE:O	5:U:177:ASN:ND2	2.49	0.42
5:U:107:ARG:HB3	5:U:109:ARG:NH1	2.35	0.42
5:U:110:HIS:CD2	5:U:145:ARG:NH1	2.88	0.42
5:U:130:ILE:HG12	5:U:131:GLN:N	2.34	0.42
2:B:24:LEU:O	2:B:24:LEU:CD2	2.67	0.42
3:H:6:GLN:NE2	3:H:107:THR:HB	2.34	0.42
3:H:127:GLY:O	4:L:213:GLU:HB3	2.20	0.42
3:H:166:PHE:HB3	3:H:167:PRO:HD2	2.00	0.42
1:A:41:HIS:O	1:A:42:CYS:CB	2.67	0.42
3:H:122:TYR:CD2	4:L:124:GLN:CG	3.03	0.42
5:U:108:GLY:HA2	5:U:110:HIS:CE1	2.55	0.42
5:U:202:THR:O	5:U:204:GLY:N	2.44	0.42
1:A:73:PRO:CD	1:A:73:PRO:O	2.68	0.42
3:H:100(A):VAL:O	3:H:100(A):VAL:HG22	2.16	0.42
3:H:134:SER:OG	3:H:185:SER:HB2	2.20	0.42
3:H:169:VAL:CB	3:H:176:THR:O	2.63	0.42
4:L:7:THR:HA	4:L:8:PRO:C	2.43	0.42
4:L:145:ASN:O	4:L:196:ALA:CB	2.63	0.42
5:U:128:HIS:CD2	5:U:142:ARG:NE	2.88	0.42
5:U:133:GLY:N	5:U:137:ARG:CZ	2.83	0.42
3:H:29:PHE:O	3:H:29:PHE:HD1	2.00	0.41
3:H:35:HIS:CG	3:H:100(B):LEU:HD21	2.54	0.41
4:L:37:LEU:HD13	4:L:86:TYR:CD1	2.55	0.41
4:L:185:GLU:O	4:L:188:ARG:N	2.32	0.41
5:U:1:LEU:C	5:U:1:LEU:HD13	2.45	0.41
5:U:77:ASN:OD1	5:U:77:ASN:N	2.49	0.41
5:U:153:CYS:O	5:U:153:CYS:SG	2.77	0.41
5:U:197:CYS:SG	5:U:239:ARG:CG	3.08	0.41
1:A:35:LYS:HG2	1:A:36:LYS:N	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HA	1:A:101:TYR:CD1	2.48	0.41
3:H:2:VAL:CG2	3:H:102:TYR:CE2	3.03	0.41
3:H:112:SER:HG	3:H:113:SER:H	1.63	0.41
3:H:123:PRO:HG2	4:L:121:SER:OG	2.20	0.41
3:H:154:TRP:NE1	3:H:163:VAL:CG1	2.83	0.41
4:L:8:PRO:HG2	4:L:11:LEU:HB2	2.02	0.41
4:L:48:ILE:HG22	4:L:49:TYR:H	1.85	0.41
4:L:81:GLU:CD	4:L:81:GLU:N	2.77	0.41
1:A:54:ASN:O	1:A:55:GLY:C	2.63	0.41
2:B:6:LYS:CE	2:B:38:GLU:CD	2.93	0.41
3:H:4:LEU:HD23	3:H:4:LEU:HA	1.88	0.41
4:L:43:SER:HA	4:L:44:PRO:HD3	1.83	0.41
4:L:179:LEU:O	4:L:181:LEU:CD1	2.67	0.41
5:U:92:TYR:CB	5:U:118:PRO:CA	2.95	0.41
5:U:97:SER:HA	5:U:145:ARG:C	2.44	0.41
5:U:222:CYS:O	5:U:265:CYS:HA	2.21	0.41
1:A:79:VAL:C	1:A:81:GLN:N	2.78	0.41
5:U:59:THR:HG22	5:U:101:SER:CB	2.50	0.41
5:U:153:CYS:O	5:U:170:CYS:SG	2.78	0.41
5:U:234:GLN:O	5:U:235:SER:CB	2.68	0.41
5:U:268:LYS:C	5:U:269:SER:O	2.60	0.41
1:A:14:LEU:HD23	1:A:41:HIS:O	2.21	0.41
1:A:60:GLY:N	1:A:103:ARG:HH12	2.18	0.41
1:A:99:HIS:CD2	1:A:99:HIS:O	2.73	0.41
3:H:34:MET:HA	3:H:93:ALA:O	2.19	0.41
3:H:41:HIS:O	3:H:43:LYS:N	2.54	0.41
3:H:100(B):LEU:N	4:L:89:TRP:HH2	2.17	0.41
3:H:134:SER:O	3:H:135:MET:SD	2.78	0.41
4:L:89:TRP:HB3	4:L:98:PHE:CE2	2.55	0.41
5:U:195:TYR:O	5:U:239:ARG:HB3	2.20	0.41
3:H:166:PHE:CE1	4:L:176:SER:CB	3.03	0.41
5:U:161:ASN:ND2	5:U:239:ARG:O	2.53	0.41
5:U:207:SER:N	5:U:208:GLU:OE1	2.53	0.41
3:H:6:GLN:NE2	3:H:107:THR:CB	2.84	0.41
4:L:89:TRP:CB	4:L:97:THR:O	2.69	0.41
4:L:193:THR:HG23	4:L:208:SER:OG	2.20	0.41
5:U:157:ASN:HB3	5:U:245:SER:HB3	2.03	0.41
1:A:51:TYR:CE1	1:A:111:PRO:HD3	2.56	0.41
1:A:79:VAL:O	1:A:81:GLN:N	2.53	0.41
3:H:39:GLN:HA	3:H:45:LEU:CD2	2.50	0.41
3:H:148:GLU:HG2	3:H:175:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:60:ASP:C	4:L:62:PHE:N	2.77	0.41
4:L:108:ARG:NE	4:L:109:ALA:O	2.53	0.41
5:U:121:GLN:O	5:U:123:LEU:HD11	2.20	0.41
1:A:74:TRP:HH2	1:A:113:CYS:HA	1.86	0.41
1:A:86:ALA:HB2	1:A:96:LEU:HB2	2.03	0.41
2:B:24:LEU:CD1	2:B:28:TYR:OH	2.67	0.41
3:H:100(B):LEU:O	4:L:46:ARG:HD3	2.20	0.41
3:H:123:PRO:CD	3:H:208:LYS:HE2	2.50	0.41
3:H:182:THR:O	3:H:183:VAL:HG13	2.21	0.41
4:L:104:LEU:HG	4:L:105:GLU:N	2.35	0.41
4:L:116:SER:HB2	4:L:118:PHE:CZ	2.49	0.41
5:U:25:ARG:HH11	5:U:27:THR:CB	2.32	0.41
5:U:40:LEU:HA	5:U:40:LEU:HD13	1.64	0.41
5:U:121:GLN:N	5:U:148:GLY:O	2.47	0.41
5:U:229:HIS:O	5:U:230:GLU:O	2.39	0.41
1:A:44:ILE:HG22	1:A:60:GLY:HA2	2.02	0.41
3:H:47:TRP:CD1	4:L:96:LEU:CB	2.95	0.41
3:H:47:TRP:HH2	3:H:58:SER:CB	2.34	0.41
4:L:4:MET:HB2	4:L:98:PHE:O	2.20	0.41
4:L:15:ILE:CG2	4:L:16:GLY:N	2.84	0.41
4:L:17:GLN:CB	4:L:18:PRO:HD2	2.46	0.41
5:U:34:GLU:CG	5:U:35:GLY:H	2.34	0.41
5:U:177:ASN:OD1	5:U:177:ASN:C	2.63	0.41
1:A:19:CYS:C	1:A:20:VAL:HG13	2.46	0.40
1:A:26:SER:O	1:A:27:ASN:C	2.63	0.40
1:A:53:GLY:C	1:A:55:GLY:H	2.29	0.40
4:L:6:GLN:OE1	4:L:100:ALA:N	2.54	0.40
1:A:61:LYS:CB	1:A:101:TYR:CD1	3.00	0.40
3:H:124:LEU:O	3:H:139:GLY:O	2.39	0.40
4:L:38:GLN:CD	4:L:44:PRO:HG3	2.44	0.40
5:U:159:PHE:CZ	5:U:161:ASN:ND2	2.89	0.40
5:U:182:LEU:HD22	5:U:187:LEU:HD11	2.04	0.40
1:A:44:ILE:HG23	1:A:59:ARG:HB2	2.03	0.40
3:H:6:GLN:HA	3:H:22:CYS:HA	2.02	0.40
3:H:125:ALA:O	4:L:119:PRO:HD2	2.21	0.40
4:L:23:CYS:CB	4:L:35:TRP:CH2	2.95	0.40
5:U:55:LEU:H	5:U:148:GLY:HA2	1.86	0.40
5:U:107:ARG:HB3	5:U:109:ARG:HH11	1.81	0.40
5:U:184:LEU:O	5:U:186:ASN:CA	2.66	0.40
5:U:218:PRO:O	5:U:243:THR:HG22	2.22	0.40
5:U:223:LEU:C	5:U:224:VAL:CG2	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:HZ	5:U:55:LEU:HB3	1.86	0.40
1:A:119:LEU:C	1:A:119:LEU:CD1	2.93	0.40
3:H:26:GLY:C	3:H:27:TYR:CD2	2.99	0.40
3:H:31:SER:O	3:H:32:TYR:CD1	2.74	0.40
3:H:37:VAL:HG21	3:H:103:TRP:CH2	2.54	0.40
3:H:68:THR:HB	3:H:81:GLN:CB	2.50	0.40
5:U:167:PHE:CE2	5:U:182:LEU:HD11	2.48	0.40
5:U:202:THR:C	5:U:204:GLY:N	2.80	0.40
1:A:57:PHE:O	1:A:59:ARG:HG2	2.21	0.40
2:B:4:SER:O	2:B:6:LYS:N	2.54	0.40
2:B:6:LYS:CE	2:B:38:GLU:OE1	2.54	0.40
2:B:15:VAL:O	2:B:15:VAL:CG2	2.69	0.40
2:B:26:SER:O	2:B:29:GLN:CA	2.70	0.40
3:H:32:TYR:CD2	3:H:96:ILE:CB	2.95	0.40
5:U:182:LEU:HD23	5:U:182:LEU:HA	1.78	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:OE1	3:H:55:GLY:O[3_555]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/135 (91%)	86 (70%)	26 (21%)	11 (9%)	0	9
2	B	38/40 (95%)	27 (71%)	9 (24%)	2 (5%)	1	15
3	H	208/228 (91%)	176 (85%)	27 (13%)	5 (2%)	4	27
4	L	216/219 (99%)	201 (93%)	13 (6%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	U	269/283 (95%)	218 (81%)	46 (17%)	5 (2%)	6	32
All	All	854/905 (94%)	708 (83%)	121 (14%)	25 (3%)	3	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	52(A)	PRO
3	H	82(B)	SER
4	L	51	VAL
5	U	185	GLU
1	A	36	LYS
2	B	8	ARG
3	H	100	SER
5	U	230	GLU
1	A	26	SER
1	A	109	ARG
2	B	9	CYS
4	L	27(E)	SER
5	U	231	PRO
1	A	11	CYS
1	A	58	TYR
1	A	77	ALA
1	A	89	SER
1	A	105	PRO
1	A	61	LYS
3	H	100(A)	VAL
5	U	67	THR
5	U	203	HIS
1	A	69	ARG
1	A	111	PRO
3	H	189	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/119 (92%)	75 (69%)	34 (31%)	0	2
2	B	37/37 (100%)	25 (68%)	12 (32%)	0	2
3	H	184/197 (93%)	135 (73%)	49 (27%)	0	3
4	L	195/196 (100%)	153 (78%)	42 (22%)	1	6
5	U	242/251 (96%)	179 (74%)	63 (26%)	0	4
All	All	767/800 (96%)	567 (74%)	200 (26%)	0	4

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	13	CYS
1	A	14	LEU
1	A	15	ASN
1	A	25	PHE
1	A	28	ILE
1	A	31	CYS
1	A	35	LYS
1	A	42	CYS
1	A	43	GLU
1	A	44	ILE
1	A	45	ASP
1	A	51	TYR
1	A	52	GLU
1	A	54	ASN
1	A	59	ARG
1	A	63	SER
1	A	64	THR
1	A	66	THR
1	A	67	MET
1	A	72	LEU
1	A	79	VAL
1	A	83	THR
1	A	84	TYR
1	A	88	ARG
1	A	92	LEU
1	A	94	LEU
1	A	96	LEU
1	A	105	PRO
1	A	117	VAL
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	123	VAL
1	A	127	MET
1	A	128	VAL
2	B	4	SER
2	B	5	CYS
2	B	9	CYS
2	B	16	ASP
2	B	20	GLN
2	B	22	ASP
2	B	24	LEU
2	B	27	TYR
2	B	31	CYS
2	B	33	THR
2	B	36	THR
2	B	39	CYS
3	H	11	LEU
3	H	13	LYS
3	H	18	VAL
3	H	19	LYS
3	H	20	ILE
3	H	21	SER
3	H	37	VAL
3	H	41	HIS
3	H	43	LYS
3	H	44	SER
3	H	48	ILE
3	H	51	ILE
3	H	62	LYS
3	H	66	ARG
3	H	69	PHE
3	H	70	THR
3	H	71	VAL
3	H	77	THR
3	H	81	GLN
3	H	82	PHE
3	H	82(A)	ASN
3	H	82(B)	SER
3	H	82(C)	LEU
3	H	89	VAL
3	H	92	CYS
3	H	96	ILE
3	H	99	HIS

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Mol	Chain	Res	Type
3	H	102	TYR
3	H	107	THR
3	H	108	SER
3	H	109	VAL
3	H	110	SER
3	H	112	SER
3	H	113	SER
3	H	120	SER
3	H	140	CYS
3	H	142	VAL
3	H	143	LYS
3	H	145	TYR
3	H	150	VAL
3	H	152	VAL
3	H	156	SER
3	H	164	HIS
3	H	178	SER
3	H	191	GLN
3	H	193	VAL
3	H	197	VAL
3	H	208	LYS
3	H	211	VAL
4	L	2	VAL
4	L	5	THR
4	L	6	GLN
4	L	9	LEU
4	L	14	THR
4	L	21	ILE
4	L	28	ASP
4	L	33	LEU
4	L	34	ASN
4	L	36	LEU
4	L	37	LEU
4	L	39	ARG
4	L	50	LEU
4	L	56	SER
4	L	60	ASP
4	L	65	SER
4	L	72	THR
4	L	82	ASP
4	L	103	LYS
4	L	106	LEU

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Mol	Chain	Res	Type
4	L	116	SER
4	L	132	VAL
4	L	134	CYS
4	L	139	PHE
4	L	142	LYS
4	L	146	VAL
4	L	155	ARG
4	L	156	GLN
4	L	161	ASN
4	L	164	THR
4	L	167	ASP
4	L	169	LYS
4	L	170	ASP
4	L	175	MET
4	L	176	SER
4	L	178	THR
4	L	179	LEU
4	L	181	LEU
4	L	195	GLU
4	L	200	THR
4	L	211	ARG
4	L	212	ASN
5	U	4	MET
5	U	6	CYS
5	U	9	ASN
5	U	12	CYS
5	U	16	GLU
5	U	17	CYS
5	U	22	ASP
5	U	29	VAL
5	U	31	LEU
5	U	32	TRP
5	U	37	GLU
5	U	38	LEU
5	U	39	GLU
5	U	46	THR
5	U	51	THR
5	U	55	LEU
5	U	59	THR
5	U	61	LEU
5	U	62	LYS
5	U	63	ILE

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Mol	Chain	Res	Type
5	U	67	THR
5	U	73	LEU
5	U	77	ASN
5	U	78	GLN
5	U	86	THR
5	U	89	ARG
5	U	93	LEU
5	U	101	SER
5	U	106	GLU
5	U	109	ARG
5	U	113	LEU
5	U	119	GLU
5	U	123	LEU
5	U	126	VAL
5	U	127	THR
5	U	131	GLN
5	U	134	GLU
5	U	159	PHE
5	U	160	HIS
5	U	163	ASP
5	U	168	LEU
5	U	170	CYS
5	U	173	THR
5	U	175	LYS
5	U	181	ILE
5	U	182	LEU
5	U	184	LEU
5	U	186	ASN
5	U	193	GLN
5	U	209	GLU
5	U	211	PHE
5	U	212	LEU
5	U	213	ILE
5	U	219	MET
5	U	222	CYS
5	U	228	THR
5	U	233	ASN
5	U	245	SER
5	U	249	HIS
5	U	252	LEU
5	U	259	ASN
5	U	266	CYS

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Mol	Chain	Res	Type
5	U	267	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	40	GLN
1	A	85	HIS
1	A	99	HIS
1	A	116	GLN
2	B	29	GLN
3	H	6	GLN
3	H	39	GLN
3	H	99	HIS
3	H	105	GLN
3	H	199	HIS
4	L	38	GLN
4	L	90	GLN
4	L	210	ASN
5	U	131	GLN
5	U	190	ASN
5	U	260	HIS
5	U	272	ASN
5	U	273	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1	6	14,14,15	0.74	0	17,19,21	3.10	8 (47%)
6	NAG	C	2	6	14,14,15	1.03	1 (7%)	17,19,21	2.15	4 (23%)
6	NAG	D	1	5,6	14,14,15	0.85	0	17,19,21	2.13	5 (29%)
6	NAG	D	2	6	14,14,15	0.50	0	17,19,21	1.32	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1	6	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	2/6/23/26	0/1/1/1
6	NAG	D	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2	NAG	O7-C7	2.68	1.29	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1	NAG	C1-O5-C5	7.99	122.89	112.19
6	C	2	NAG	C1-O5-C5	-6.89	102.96	112.19
6	D	1	NAG	C3-C4-C5	6.15	121.38	110.23
6	C	1	NAG	O5-C5-C6	-4.87	98.19	107.66
6	C	1	NAG	C1-C2-N2	-4.75	102.94	110.43
6	D	1	NAG	C1-O5-C5	-4.29	106.43	112.19
6	C	1	NAG	C8-C7-N2	-4.23	109.10	116.12
6	D	2	NAG	C1-O5-C5	3.75	117.21	112.19
6	C	2	NAG	C2-N2-C7	-3.14	118.69	122.90
6	C	1	NAG	O6-C6-C5	-2.69	102.16	111.33
6	D	2	NAG	O5-C1-C2	2.69	115.45	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1	NAG	O4-C4-C3	-2.55	104.36	110.38
6	C	1	NAG	O4-C4-C5	2.55	115.60	109.32
6	D	1	NAG	C4-C3-C2	2.52	114.72	111.02
6	C	2	NAG	O5-C1-C2	-2.52	107.39	111.29
6	C	1	NAG	O7-C7-C8	2.52	126.53	122.05
6	D	1	NAG	O4-C4-C5	-2.35	103.54	109.32
6	D	1	NAG	O5-C5-C6	2.14	111.83	107.66
6	C	2	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

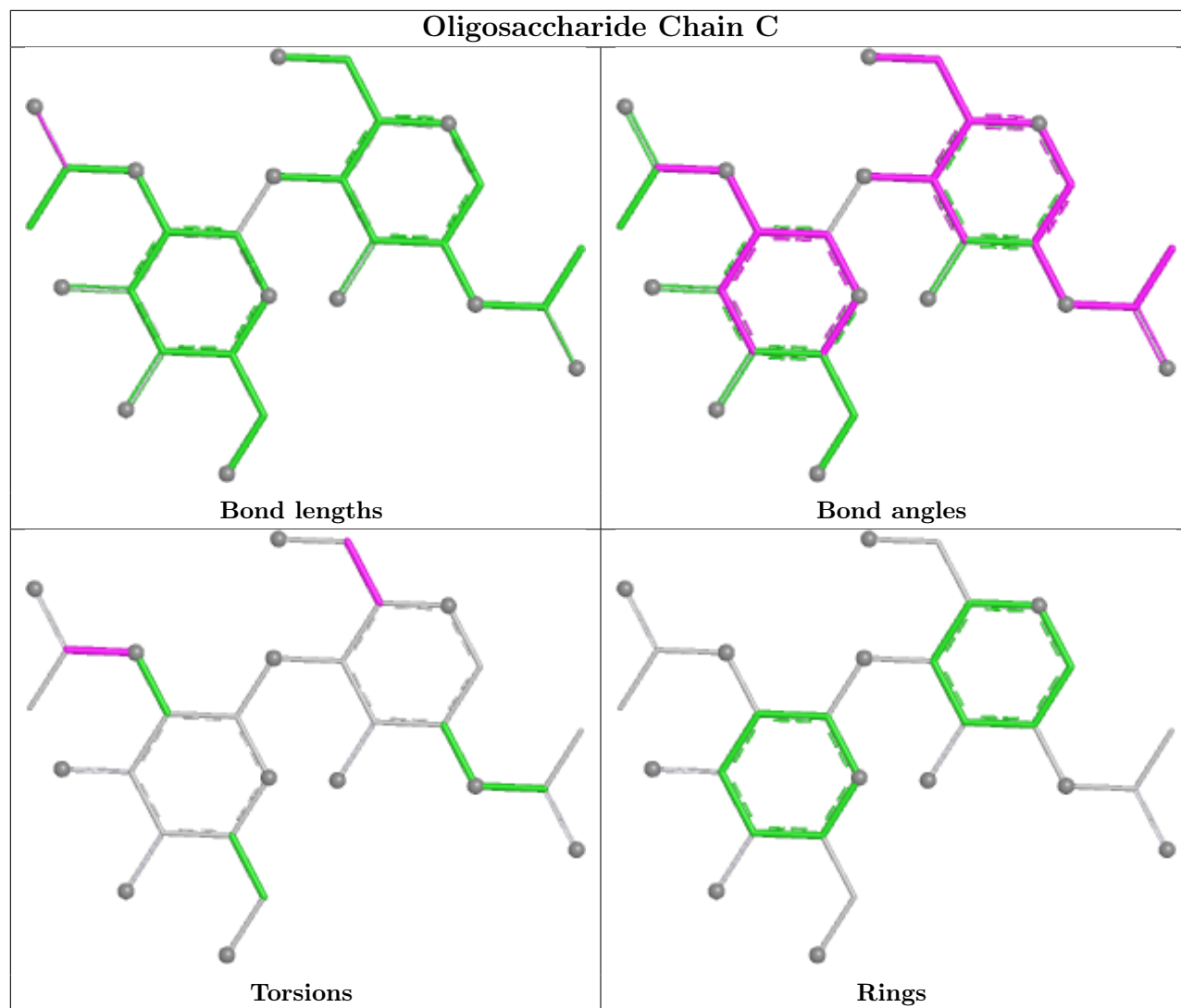
Mol	Chain	Res	Type	Atoms
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2
6	C	1	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2

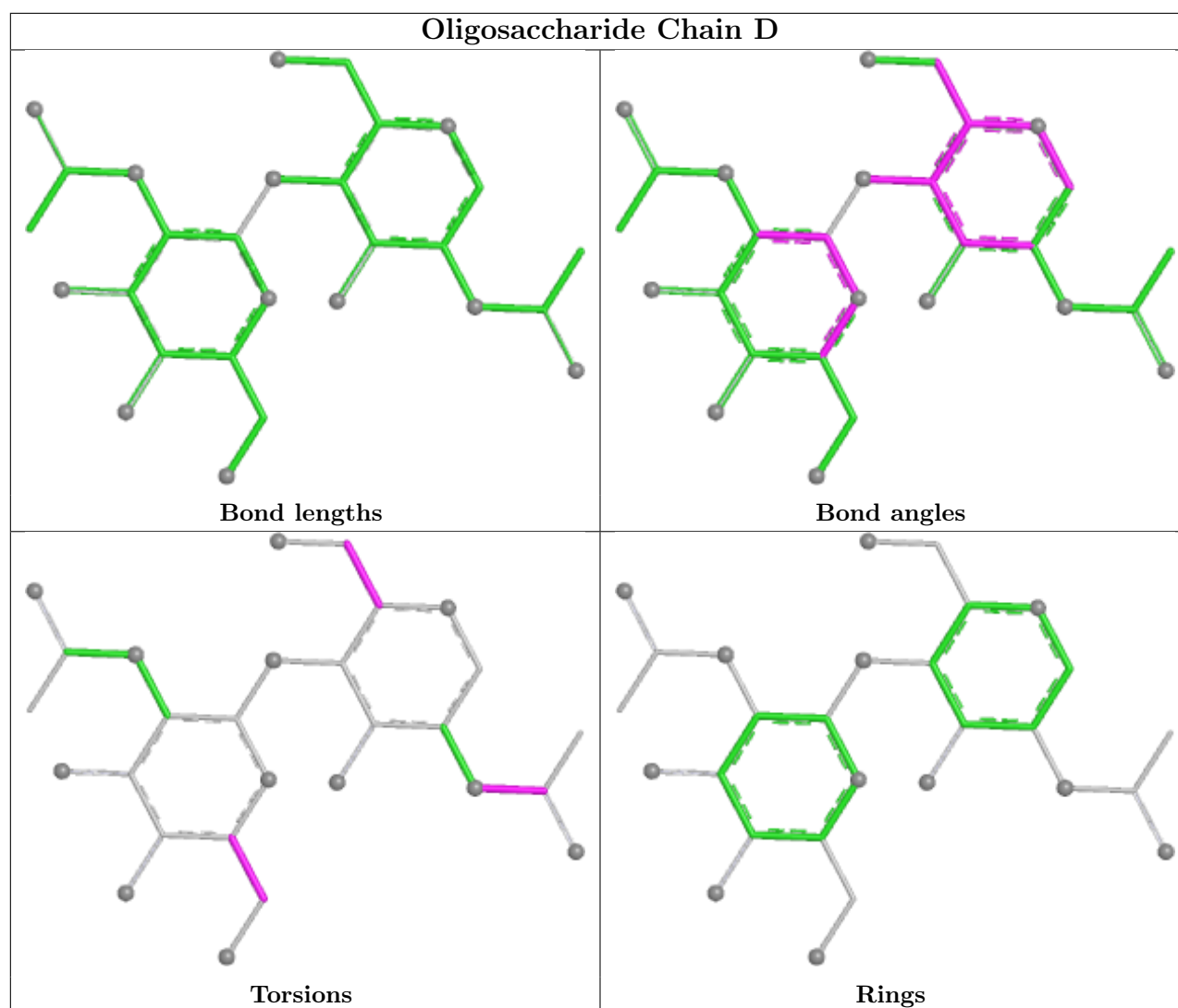
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2	NAG	3	0
6	D	1	NAG	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	U	304	5	14,14,15	0.63	0	17,19,21	1.22	2 (11%)
7	MAN	U	303	-	11,11,12	2.36	2 (18%)	15,15,17	2.75	8 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	U	304	5	-	3/6/23/26	0/1/1/1
7	MAN	U	303	-	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	303	MAN	O5-C5	5.22	1.53	1.43
7	U	303	MAN	C4-C3	-4.95	1.39	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	303	MAN	C1-C2-C3	5.57	117.76	109.64
7	U	303	MAN	O5-C5-C6	4.88	117.16	107.66
7	U	303	MAN	C1-O5-C5	3.79	117.27	112.19
7	U	303	MAN	O3-C3-C4	-3.46	102.21	110.38
8	U	304	NAG	C3-C4-C5	3.16	115.96	110.23
7	U	303	MAN	O6-C6-C5	2.78	120.81	111.33
7	U	303	MAN	O2-C2-C3	-2.73	104.50	110.15
8	U	304	NAG	C4-C3-C2	2.53	114.73	111.02
7	U	303	MAN	C6-C5-C4	-2.23	107.54	113.02
7	U	303	MAN	O5-C5-C4	2.05	115.83	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	U	304	NAG	O7-C7-N2-C2
7	U	303	MAN	O5-C5-C6-O6
8	U	304	NAG	C8-C7-N2-C2
7	U	303	MAN	C4-C5-C6-O6
8	U	304	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	U	304	NAG	1	0
7	U	303	MAN	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	125/135 (92%)	-0.17	2 (1%) 70 55	171, 240, 348, 489	0
2	B	40/40 (100%)	-0.17	0 100 100	226, 301, 419, 468	0
3	H	212/228 (92%)	-0.19	2 (0%) 81 67	187, 291, 431, 531	0
4	L	218/219 (99%)	-0.13	0 100 100	220, 335, 449, 596	0
5	U	273/283 (96%)	-0.20	2 (0%) 84 71	192, 290, 443, 635	0
All	All	868/905 (95%)	-0.18	6 (0%) 84 71	171, 296, 440, 635	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	127	GLY	3.3
5	U	207	SER	3.0
3	H	120	SER	2.4
1	A	43	GLU	2.1
5	U	268	LYS	2.1
1	A	40	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

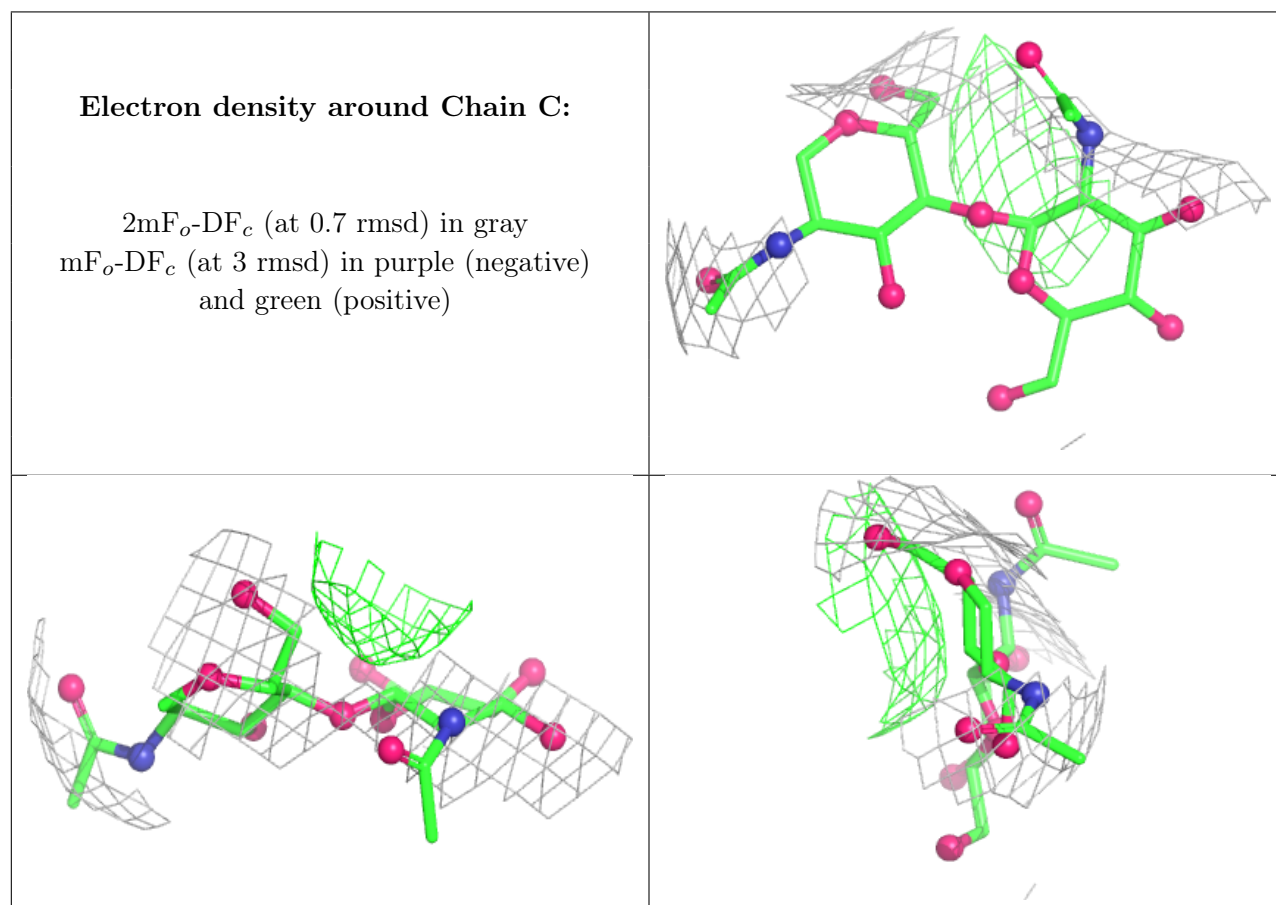
There are no non-standard protein/DNA/RNA residues in this entry.

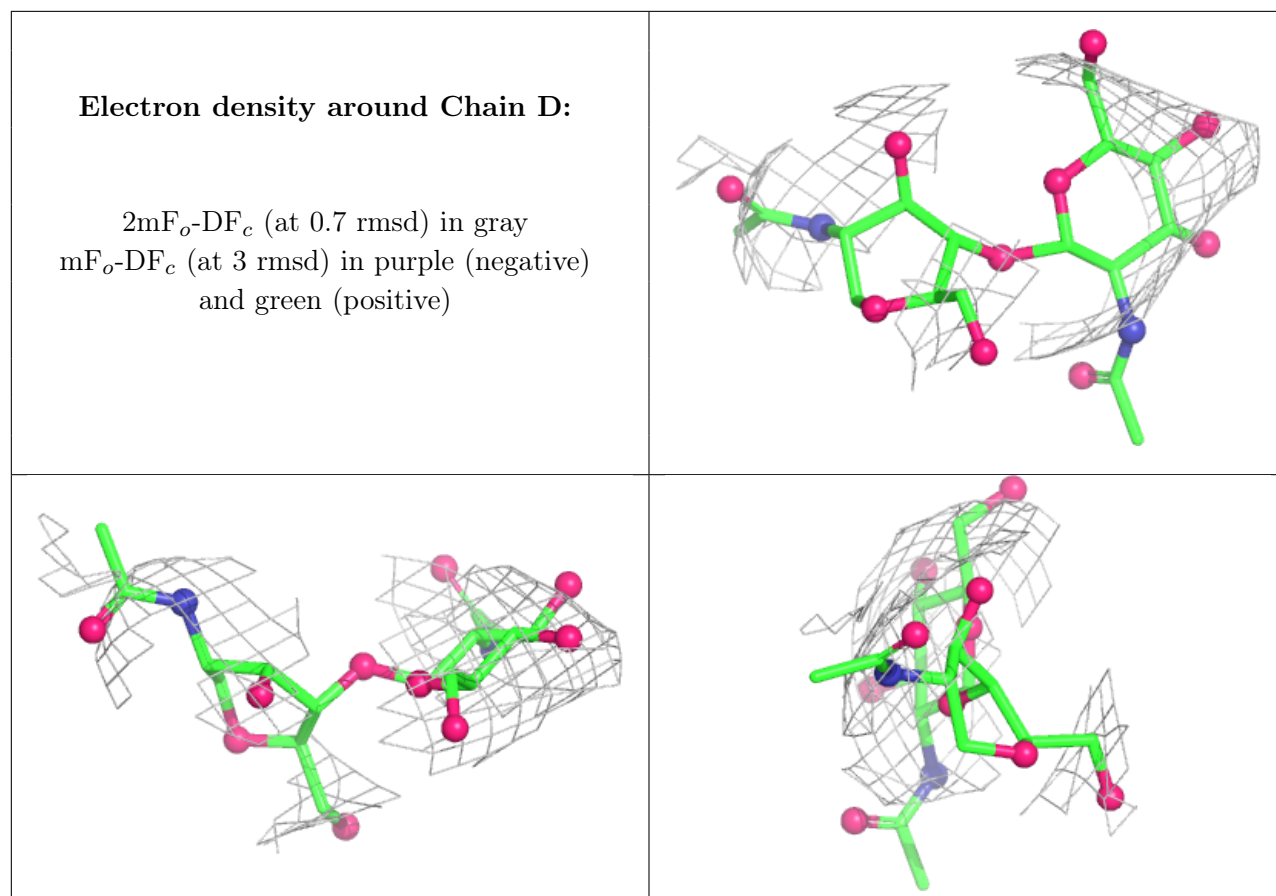
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	C	1	14/15	-	-	281,296,310,313	0
6	NAG	C	2	14/15	-	-	443,452,459,461	0
6	NAG	D	1	14/15	-	-	444,446,448,449	0
6	NAG	D	2	14/15	-	-	449,453,455,456	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MAN	U	303	11/12	0.61	0.08	404,442,450,450	0
8	NAG	U	304	14/15	0.79	0.14	492,494,498,498	0

6.5 Other polymers [i](#)

There are no such residues in this entry.